Guide to the XAFS Data Acquisition Software at PNC-CAT BM20/ID20

Last updated: February 11, 2003

1. Introduction

This document is an informal guide, written from the viewpoint of a beamline (BL) user, to the XAFS software and BL control suite on the PNC-CAT BM20/ID20 BL, which are located at the Advanced Photon Source (APS).

After you arrive at APS, the BL staff will set up the BL equipment so that it is ready for your XAFS (X-ray absorption fine structure) measurements. They will show you how to mount and change samples inside the BL hutch, and how to operate the XAFS data acquisition software. Subsequently you will be left to carry out XAFS measurements by yourself as far as possible. The BL staff will be available for consultation if problems arise, or if you do not know (or forget) how to do something.

The main operations which have to be completed by a user after mounting a new sample may be summarized by the following list:

a) Set widths of I_0 slits
b) Set sample (x, y) position
c) Set scan configuration
d) Set amplifier sensitivities
e) Set data storage information (folder, file group name, comments)
f) Set number of scans
g) Initiate a simple scan or a program of scans

The following sections of this document contain task-oriented descriptions of these operations ('how do I do this?'). In contrast, the Appendix contains a module-oriented description ('what does this do?') of the parts of the software suite which might be of interest to users (some of the software controls elements of the BL hardware which users do not need to know about, and should avoid disturbing). The guide assumes that the software modules which you need for each task are already open on the desktop, or that you know how to access them. But they may not be, or you may have accidentally closed (and lost) them. If so, refer to the Appendix to locate them.

Note that much of the software is similar or identical on both the bend magnet (BM20) and insertion device (ID20) stations. Many of the same tricks are or can be done at either station. The principle difference is in what experiments are more likely to be done at the station. The following sections labeled ID or BM are those experiments most likely done at those stations. If an experiment is not in that section it may be in the other section. The Appendix contains many menus that are common to both stations. Also note that in some cases the only difference between the software at the stations is a label of either BM or ID.

1.1. Detectors and Sensitivity Settings

The simplest detectors used on the both beamlines are ion chambers in the beam. These are typically used for measuring I0 and I1. There are displays of these detectors which tell you the current signal. These are useful to watch when making any adjustments to the setup.

- Set sensitivity for the usual "scalar" channels (ion chambers and the like) so that reading is ~ 3v

- A value of 7 specifies saturation, it may be much bigger than this so absolute signal is greatly attenuated
- I_1 may be simple transmission or it maybe called I_2 and I_2 sometimes called I-trans!!!
- I_0 is generally always labeled as such.

Caution: make sure you have correctly linked/labeled detectors so that it is clear which signal is coming in and what it is called. Labels may not always match. This is particularly true in the software where channel names may not match the input device. It is up to the user to name/label inputs in a consitent/logical manner.

In general make sure you know where in the stream it is measures and how (ion chamber, pin diode, etc).

Detectors that are listed as 'scalar' detectors include simple Lytle Type, TEY (Total electron yield) and pin diode fluorescence detector.

Fluorescence is also recorded by single component (element) solid state detector or multicomponent (ex. 9 elements, 13 elements, etc) solid state detector. See MCA directions for further information.

2. The BM20 data acquisition system desktop

Fig. 1 shows the desktop on the computer which is used to acquire XAFS data. It runs a familiar Win32 operating system. Typically the desktop presents a cluttered view, with many open programs (not all of which may be relevant for your purposes).

The computer runs a desktop management program called WinSpace which creates a number of so-called 'virtual screens' on to which running programs may be dragged. You can display a virtual screen on the main screen by clicking (with the mouse) the relevant rectangle of the WinSpace display. This will hide all programs from the current display. By distributing different programs among the five WinSpace screens you can reduce desktop clutter on the main screen.

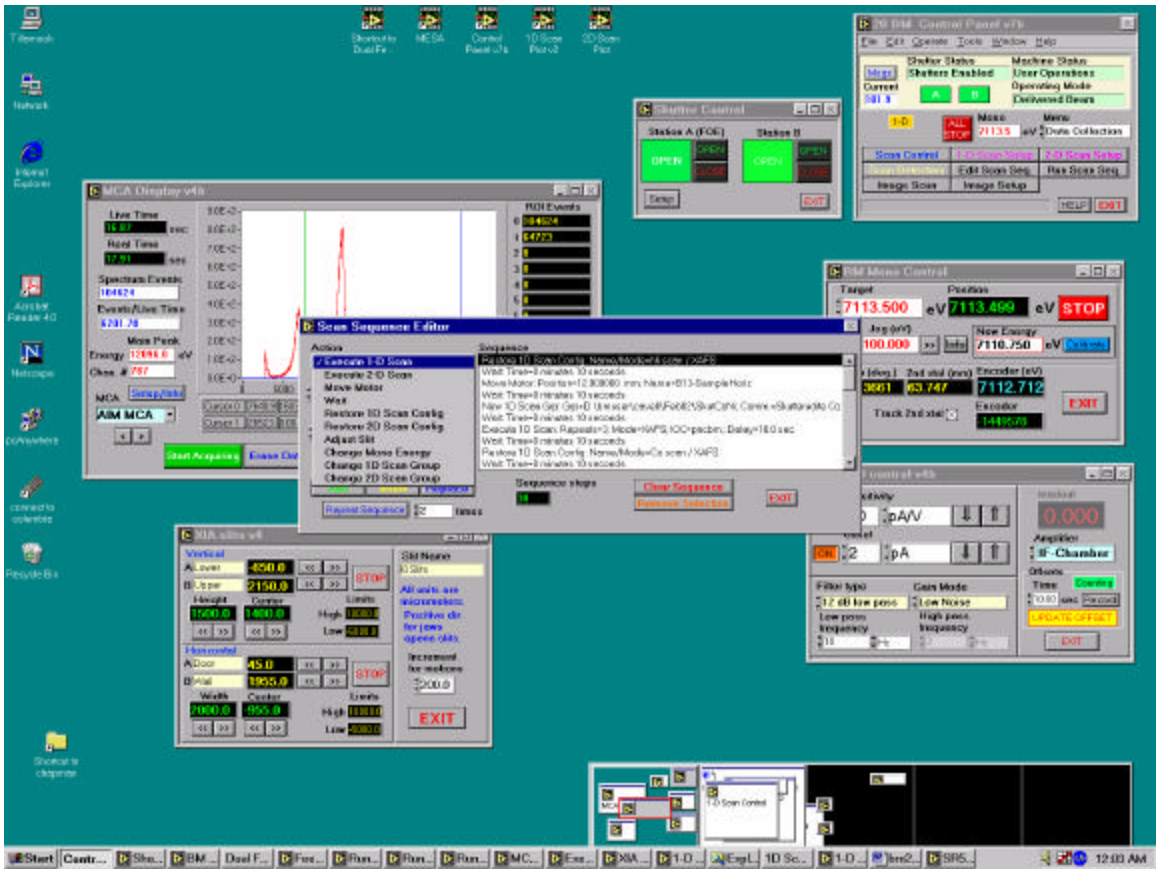


Fig. 1. View of the BM20 data acquisition system desktop. The rectangular areas at bottom left are the WinSpace virtual screens.

3. BM User tasks

3.1. Set widths of I_0 slits

Fig. 2 shows the **XIA Slits** dialog box which is used to change slit widths. This is not a frequent operation, but some samples may require it. The caption of the figure explains how to make the adjustment. The slits define the shape of the beam which is allowed to enter the ionization chamber just in front of the sample (I_0 refers to the current measured by this chamber, which is used as a photon flux normalization reference for XAFS spectra).

Typical maximum values for the slit widths are 3000 (horizontal) and 1500 (vertical), both measured in microns (?m). There is no point in opening up further than this. However, under some circumstances you may wish to narrow the slits, e.g. to study a small region of the sample.

The effect of reducing the slits is to reduce the photon flux impinging on your sample. You can see the effect of this by looking at the 'I0 Monitor' output which is displayed on the rack near the computer.

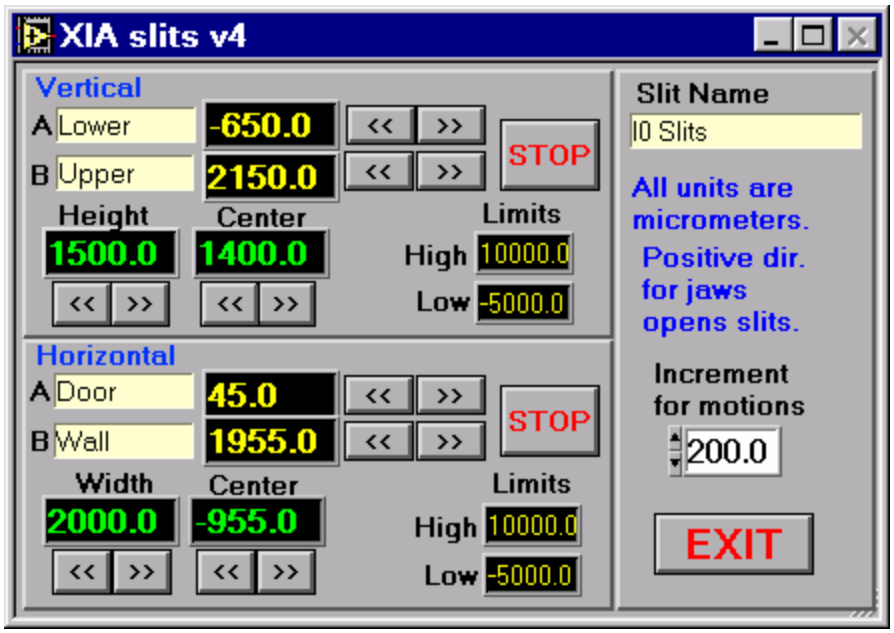


Fig. 2. Set widths of I_0 slits. All units are microns (1000 ?m = 1 mm). Note **Slit Name** at top right – there are other slits in the system which you should not change. Under normal circumstances, users should only modify the Height and Width settings. This is achieved by clicking the **Increase** [>>] and **Decrease** [>>] width buttons on the vertical and/or horizontal slits. **EXIT** will close the dialog box, while **STOP** will halt the operation.

3.2. Set sample (*x*, *y*) position

The sample (*x*, *y*) position is modified by defining new coordinates which are set up by the mechanical drives (translators). Fig. 3 shows the dialog box for the horizontal (*x*) and vertical (*y*) translations. These will normally be open somewhere on the desktop. Note the description of the motors (e.g. B13-SampleHoriz) which identifies which is which.

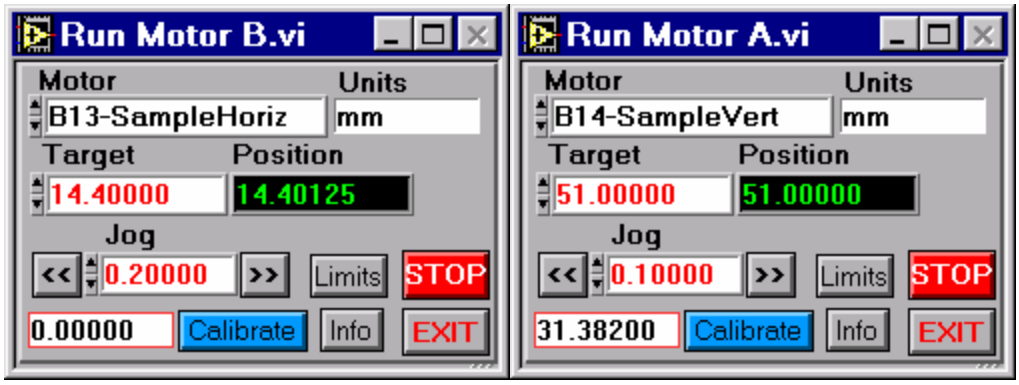


Fig. 3. Set sample (*x*, *y*) position (left: horizontal position; right: vertical position). You can either set a **Target** value (followed by the enter key), or **Jog** the position by the stated amount (which you can modify) using the arrow buttons [>>] and [<<].

3.3. Set scan configuration

The scan configuration defines the scan intervals, scan rate, and scan ranges of your XAFS measurement (intensity versus photon energy), which in BM20 terminology is known as a 1-D scan. The 1-D scan set-up is shown in Fig. 4, the caption of the figure explains how to do the set-up.

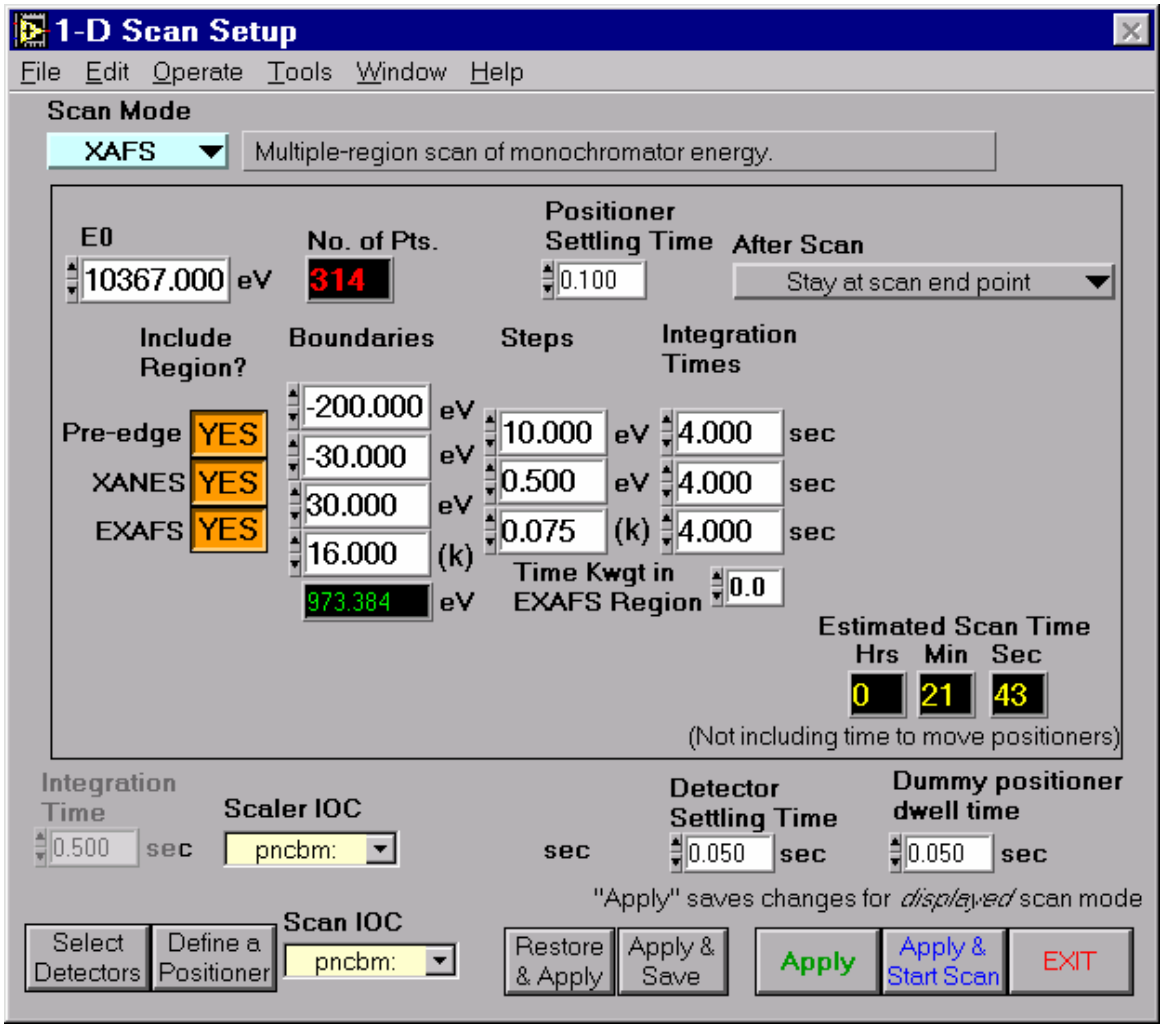


Fig. 4. Set scan configuration (XAFS scans are known as 1-D scans at BM20). The user must provide values for the step edge (**E0**), the **Boundaries** of the ranges, the sizes of **Steps**, and the **Integration Times**. The values shown are for Ga. The **Integration Times** are often 1 or 2 s, rather than 4 s as shown here. Otherwise, the values are the standard ones which you will probably use yourself. (Often only **E0** is changed from scan to scan.) Note that the upper limit of the EXAFS range is expressed in terms of the wave-vector, **k**, ranging here up to 16 $Å^{-1}$ (k = 0 is assumed to coincide with **E0**). The corresponding energy width in eV is listed below the input box (973 eV). Other parameters should be left at their default values. Changes made to this dialog box are not transferred to the system until you click the button which has the word

Apply in its caption. A red text message will come up when you edit any parameters to advise you that the changes have not been applied.

A scan set-up must be explicitly applied before it is 'known' to the system. If you modify a setting and press exit, the next scan will continue to use the old scan settings. Scan set-ups can be saved to, or read from, the computer disk. A maximum of 10 set-ups is allowed, and usually all 10 have will already been defined by previous BL users. You will have to select an existing set-up, and replace it, if you wish to save your own settings (**Apply & Save** command). This command brings up an unnecessarily alarming orange-coloured warning box (telling you that 10 set-ups are already defined), which you can ignore.

In summary, use the button commands at the bottom of the dialog box to:

? Read and apply a setup (**Restore & Apply**)
? Apply the set-up and then save it (**Apply & Save**)
? **Apply** the set-up (but don't save it)
? Apply the set-up, and then start the scan (**Apply & Start Scan**)
? **Exit** (but don't apply)

XAFS scans are divided into 3 regions (pre-edge, XANES, EXAFS), which are scanned differently. You can disable any of the region scales by depressing the **YES** buttons shown in Fig. 4. The standard scan mode scans EXAFS spectra on a linear range in *k*-space. The scan shown in Fig. 4 uses energy intervals of about 2-8 eV; the intervals increase as the scan moves further from the edge.

3.4. Set amplifier sensitivities

The need for this operation arises because the amplifiers are not linear over their full range. It is necessary to set their sensitivities so that the signal received from your sample falls in the middle of the amplifier working range. Fig. 5 shows the SR570 control dialog box which is used for this task, and explains what is involved. It will be necessary to check or set the sensitivity for every amplifier which you are using (including the I_0 amplifier). Typically, that means setting 3-4 amplifiers: I_0, I_2, (transmission), fluorescence, TEY. In practice the I_0 sensitivity does not need adjusting very often. To prevent the output falling to near zero, an offset of 10% is added once the sensitivity range has been determined.

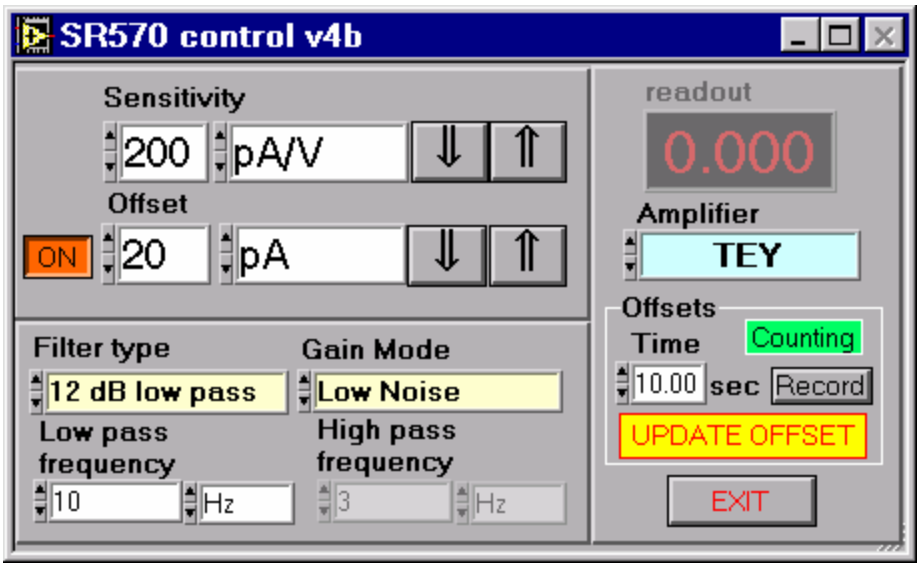


Fig. 5. Set amplifier sensitivities. First you must select an amplifier from the set which you are using: the **TEY** amplifier (used for total electron yield measurements) is indicated here. Then move the mono (monochromator) to the energy region(s) where you want to test the response (see Fig. 6), and adjust the sensitivity so that the readout never exceeds about 3.0 V (lower readouts, 1.0-2.0 V, are adequate). These energy regions are those in which you expect to get the highest amplifier response. Except for transmission data (I_2) this corresponds to the region above the absorption edge. The I_2 amplifier sensitivity should be set up in a region *below* the edge. Set the offset to 10% of the sensitivity range value (as shown in the figure). Other parameters should be left at the default values. After changing sensitivity or offset the 'UPDATE OFFSET' warning comes on. With the shutter closed, press **Record** to update. This will update all of the amplifiers.

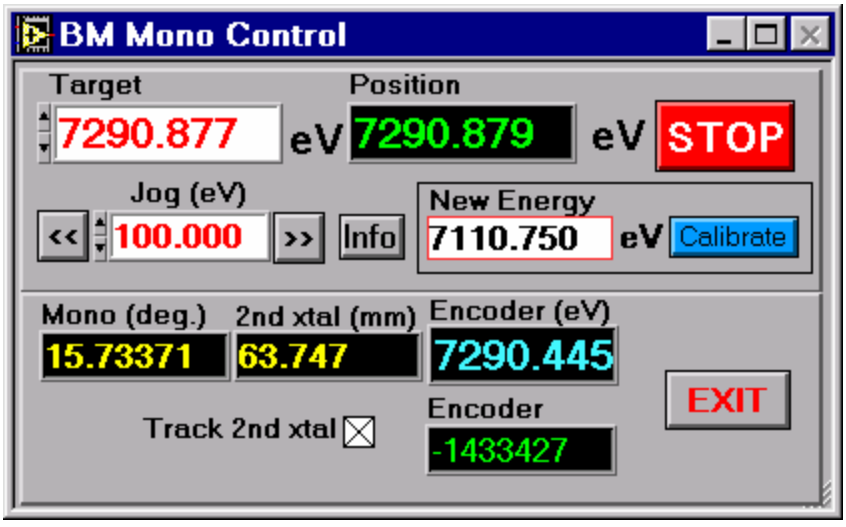


Fig. 6. Monochromator control. This control is used to manually adjust the current photon energy by changing the double crystal monochromator settings. You can select a **Target** energy, or you can **Jog** the monochromator by the amount specified. For example, you could move to an energy of ~8000.0 eV by entering '8000', or by hitting the **Jog** [>>] button 7 times in succession. If you choose to make a large move (1000 eV), you will be prompted for confirmation ('Whoa, Nelly!'). A move operation can be aborted by clicking **STOP**. The option to **Track 2nd xtal** (crystal) should be set as shown [X]. If you switch it off, the beam will switch to a different position on the second monochromator crystal. Sometimes this is beneficial (e.g. if that spot happens to be bad), but usually this is avoided. Other buttons/parameters should not be clicked/adjusted by users.

3.5. Set data storage information

At this stage you should locate the 1-D scan control dialog box (Fig. 7).

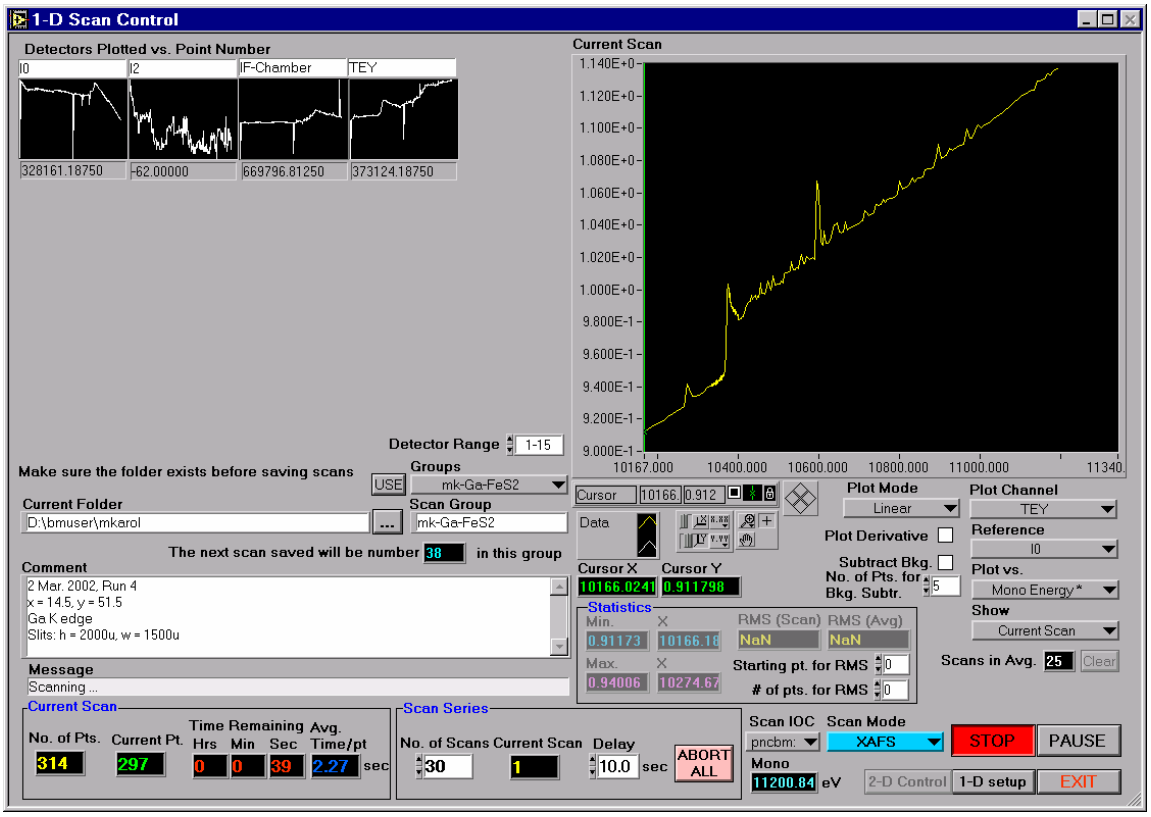


Fig. 7. 1-D Scan Control dialog box. This is the main window which you will use for monitoring the progress of XAFS scans. Most of the controls below the large chart on the right are concerned with how the data are displayed. The **STOP** button stops the current scan and moves to the next scan. It becomes a green **START** button when scanning is complete. To stop all scans, click **ABORT ALL**, or set the **No. of Scans** to the same value as the **Current Scan** index. **Pause**/**Resume** allows you to pause the scan and then resume.

Before starting the scan, you must specify the folder (which must exist before the scan starts), and enter a file group name, as well as any comments which you wish to attach to the data files. These tasks are straightforward, so long as you understand the file naming convention used by the software:

? **Current Folder**: folder in which data are stored (select via […] button).
? **Scan group**: stem of data file names. For example, if the scan group is specified as **test** then scan 1 will be saved as **test.0001**, scan 2 as **test.0002** etc. You can either define a new name, or use an existing group name (see next item)
? **Groups**: brings down a list of the scan groups found in the folder specified. If you choose one and press 'USE', the name will be transferred to the scan groups edit box. The next scan will be assigned the first free index number e.g. if **test.0009** is the last existing file in the group, the next spectrum you scan will be named **test.0010**.

3.6. Set number of scans

The **No. of Scans** parameter determines how many scans will be accumulated. It can be increased or decreased while the spectrometer is running. The **Current Scan** index indicates the progress of the scanning procedure during data measurement. The message **The next scan saved will be number XX in this group** indicates the number that will be attached as an extension to the data file (e.g. **test.0024**); if this is the first time you are using this group it will be identical to the current scan index.

3.7. Initiate a simple scan

Simple scans which involve a fixed set of parameters are initiated by clicking the **START** button in the 1-D Scan Control dialog box (see Fig. 7). The scan will follow the specifications defined in the 'set scan configuration' stage (section 3.3). You can stop, pause, restart or abort the scan. Each time a new scan starts, it will produce a data file with a unique name (e.g. **test.XXXX**, where the digits XXXX number the file). There are many other (optional) data display features of the 1-D Scan Control box. One useful feature which should be mentioned here is the **Show** option which allows you to display averaged spectra and/or the current scan. To use this feature, you must click the **Clear** button before the scan starts. This sets the accumulator to zero (clears previously collected data). The button is disabled during scanning.

3.8. Initiate a program of scans

Scans may be programmed. The program is specified via the Scan Sequence Editor (Fig. 8). The (blue) drop-down list provided under the **Action** field allows the user to select a series of operational steps (actions) and their accompanying parameters. It is recommended that after each action you insert a wait statement of about 10s which will allow the system to settle down.

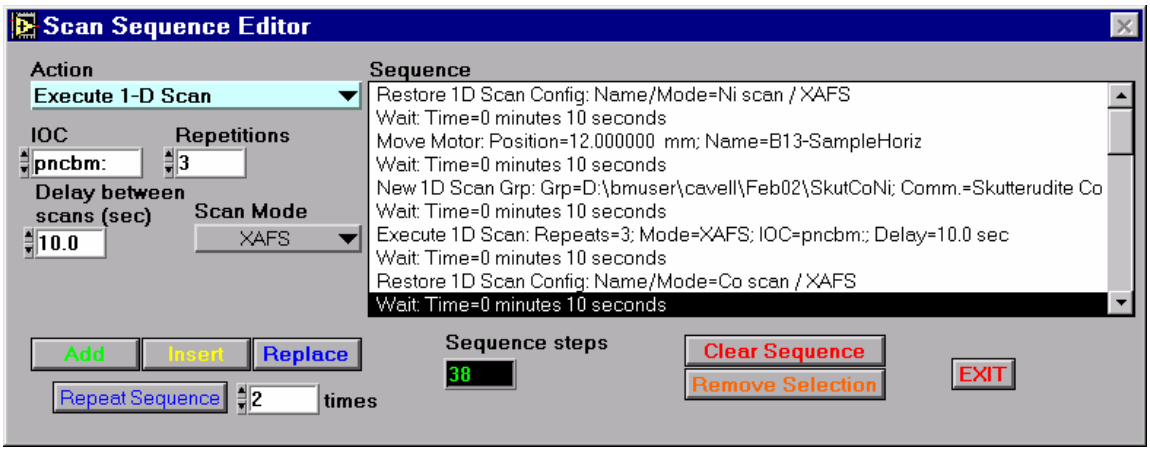


Fig. 8. Scan sequence (i.e. scan program) editor. The actions are selected and defined by the controls on the left side of the window. An action can be **Add**ed at the end of the existing sequence, **Insert**ed above the current position of the selection bar (black), or used to **Replace** an existing action. **Clear Sequence**: deletes all actions from the editor; **Remove Selection**: deletes the action under the selection bar; **Repeat Sequence**: duplicates the current sequence of actions *N* times, and appends them to the editor (this is very useful for writing long programs).

Most of the set-up operations described in preceding sections can be programmed. This is useful if you have to execute a sequence of highly repetitive tasks (e.g. scan three points on the same sample, or scan 4 elements on the same sample). However, the sensitivity settings of the amplifiers cannot be programmed. This restricts the use of programmed scans to jobs which have mutually compatible sensitivity settings.

Once you understand how to set up a simple scan, the individual programmed scan operations are quite easy to understand. However, as with all programming tasks, it is easy to do things in the wrong order. To reduce complexity, the following approach is suggested:

? Write the scan sequence for a single scan job, without using wait statements.
? After reviewing the program for correctness, insert wait statements after each action.
? Use the **Repeat Sequence** command to generate the number of scan jobs which you require.
? Make changes as necessary to actions in the program using the **Replace** function.

The program may be executed by clicking the Start Sequence button which is found on the Execute Scan Sequence window (Fig. 9). The button controls are self-explanatory (**Abort Sequence** will halt the execution of the sequence).

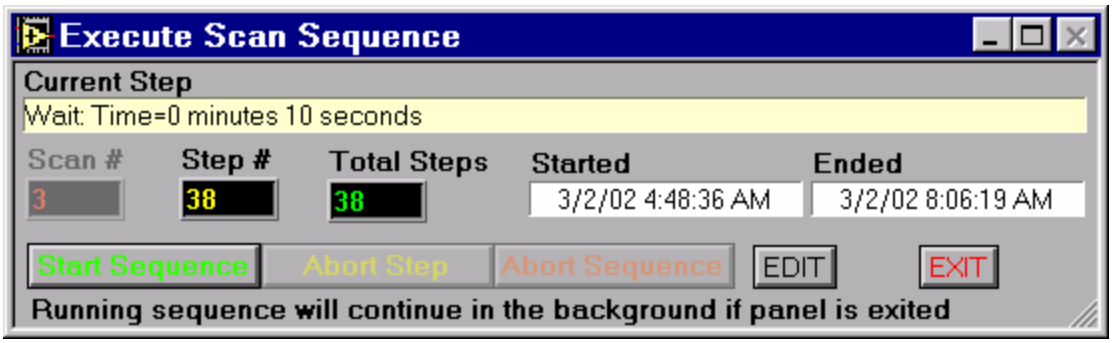


Fig. 9. Execute scan sequence window. The **Start Sequence** button will initiate the execution of the sequence (program) in a step-by-step fashion.

3.9. Display a scan

Fig. 10 shows the 1D scan plot window which can be used to display and print XAFS scan data files.

a) Select **Current Folder for Scans**, (button marked […]), and **Scan Group** of interest (via the drop down window). NB. the Scan Group information is only updated when you hit the update button.
b) Set the number of the scan (i.e. scan 1 of scan group **test** refers to the file **test.0001**).
c) Set the **Columns** to plot (**View Column Labels** will list the file format if you are uncertain).
d) Don't forget to set the **Ratio Type** (**linear** for fluorescence or TEY spectra, or **log** for transmission spectra) and **Ref**erence (I_0) column.
e) To plot the spectrum alongside the existing plot click **ADD**, or click **REPLACE** to plot the spectrum by itself. If using the **ADD** option, note the **Scale to 1st Plot** option, which you will probably use.
f) **View File Header** provides information about the data file, including user comments.

In the analysis box, there are various quick data processing options (intended to help the user assess the quality of the data). These operations (if you wish to use them) are accessed via the drop down box, e.g. Quick EXAFS in Fig. 10. You can use this option to extract some EXAFS oscillations, e.g. to assess the signal/noise ratio, or to compare data from two sources.

The buttons and labels just below the plot (**RESET PLOT**, **Cursor 1** and **Cursor 2** etc) are used for data display purposes. It probably better to explore these by yourself. These controls provide data display and exploration capabilities, e.g. area zooming, coordinate mapping.

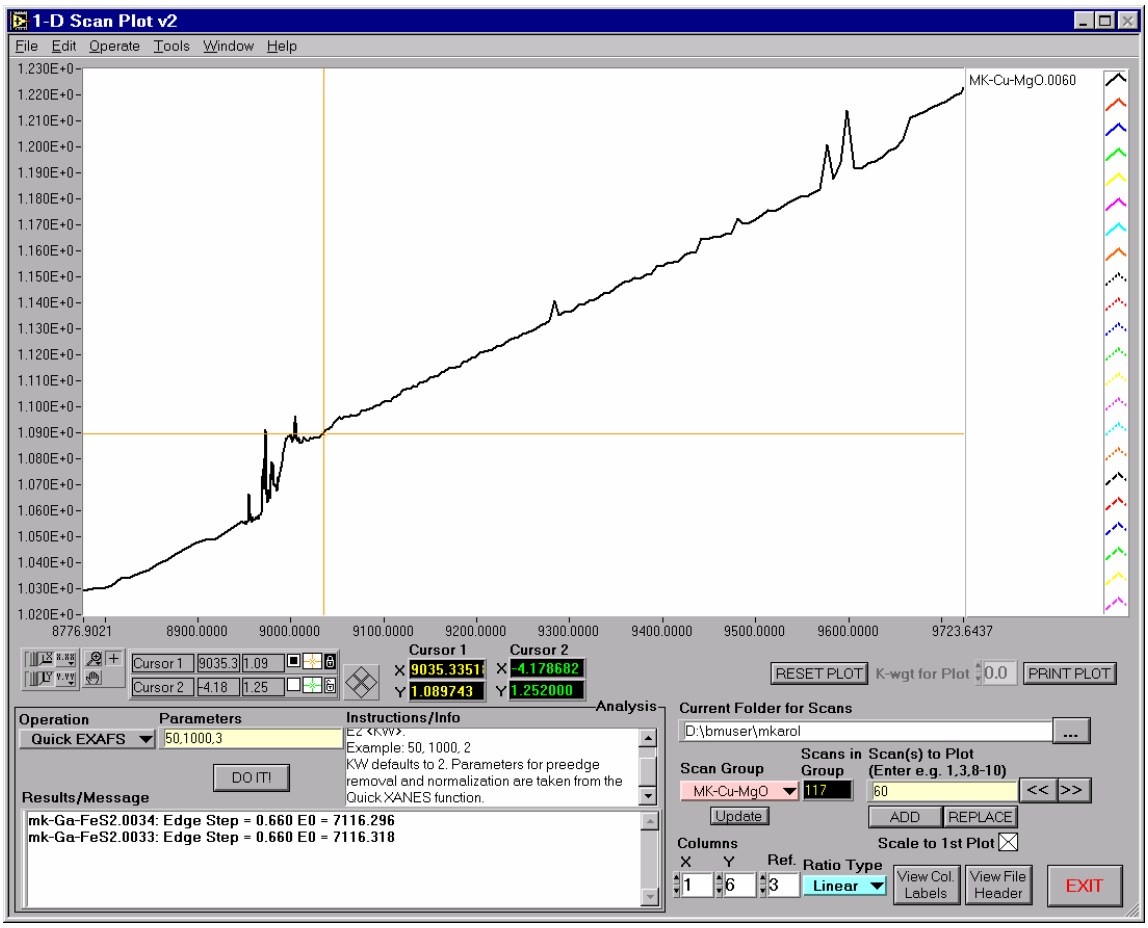


Fig. 10. 1D scan plot window which is used to display and print XAFS spectra.

4. ID 20: Production of a 2-D scan

Abbreviations

2-D	two dimensions
ID	insertion devices
ROI	regions of interest
MCA	multiple channel analyzer
Proc. Vars.	process variables

4.1. Description

A 2-D scan is a map of elemental abundance within a selected rectangular area of the analytical sample. The user can collect data on several elemental peaks during one 2-D scan by specifying several regions of interest (ROI) from a spectrum generated prior to map production. A 2D scan is most productive when the sample has been analyzed with other types of spectroscopy or examined by optical microscopy. 2D scans are a useful tool to identify interesting points for further EXAFS study. Caution should be exercised however as 2D mapping can consume much of the available beamtime.

Many of the set-up procedures are identical to those undertaken on the BM beamline, and it is suggested that the user read BM sections of this manual..

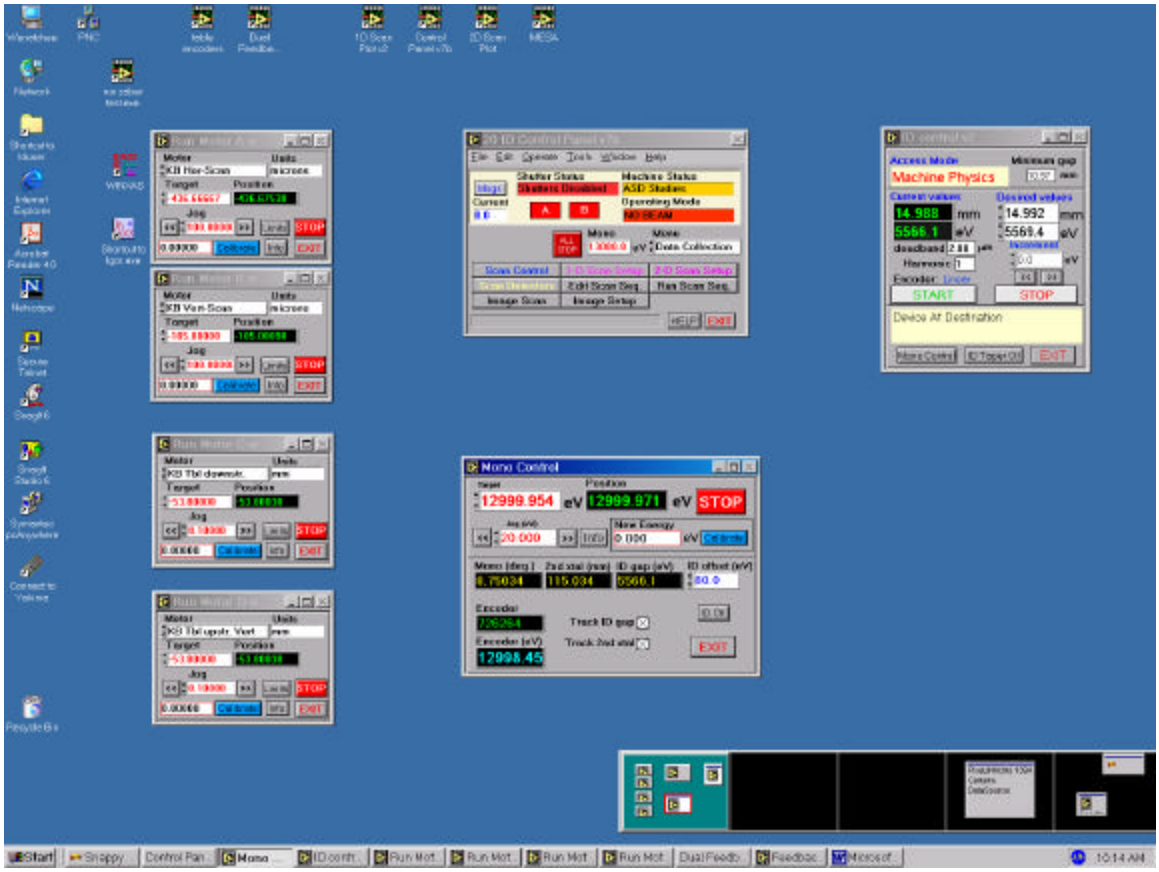
This guide is intended as a work in progress, basic step-by-step guide to the manipulation of the computer software in the production of a 2-D scan and assumes that the analytical sample has been prepared, mounted within the beamline assembly, and properly lit.

The identification of any errors in this text, or suggestions for its improvement would be gratefully received.

4.2. Active desktop configuration.

The production of a 2-D scan requires the user to specify various parameters before the scan can commence e.g. specifying the co-ordinates of the area to be mapped, setting the amplifier sensitivities etc. Therefore, at any one time during the procedure, the user will often find it easier to have several windows open, see **Fig 4.1.** In the bottom right of the screen five Winspace panels are visible. Four are black (inactive) and one is blue (active). The user can activate any panel by clicking on the black portion. The user can bring all the windows required at any stage in the procedure into a single panel by clicking and dragging the windows. Visible on the desktop are some of the windows for the program. Some of the following is identical to that described in the BM section above and some is described in the Appendix section of this manual.

Figure 4.1: ACTIVE DESKTOP CONFIGURATION



4.3. Check beamline orientation

Reason

To ensure accurate positioning of the beam and determination of the area to be mapped.

Action

Tape fluorescent or photographic ('burn') paper to the mount, ensuring that the paper is attached securely, and that it lies flat on the sample surface.

Open the beamline and record the beam dimensions on the screen in the console area by drawing around the beam rectangle using **non**-permanent marker.

(If this paper were also gridded you could confirm the actual dimensions of the beam as recorded on the screen).

Alternatively, phosphor can be placed around the sample to check the beam position but moving the beam over the phosphor. This assumes that the phosphor is at the same plane as the sample. As the sample is moved the apparent position of the beam will move outside of the

marked box due to parallax. However, you can check the horizontal and vertical positions separately.

Ideally the cross-hairs on the screen should tally with the beam position. If the screen cross-hairs and the beam are in widely different positions, the user MAY consider CAREFULLY altering the camera position.

The beam takes several minutes to affect the burn paper but the result is more accurate than a determination using fluorescent paper.

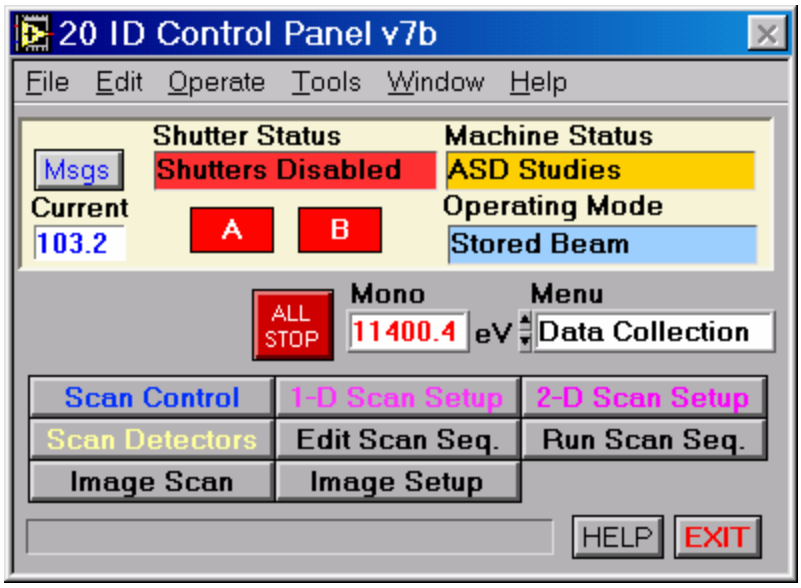
Carefully remove the burn paper without disturbing the position of the mount or sample.

4.4. Defining the area to be mapped

Reason
To provide the co-ordinates of the rectangular area to be mapped.

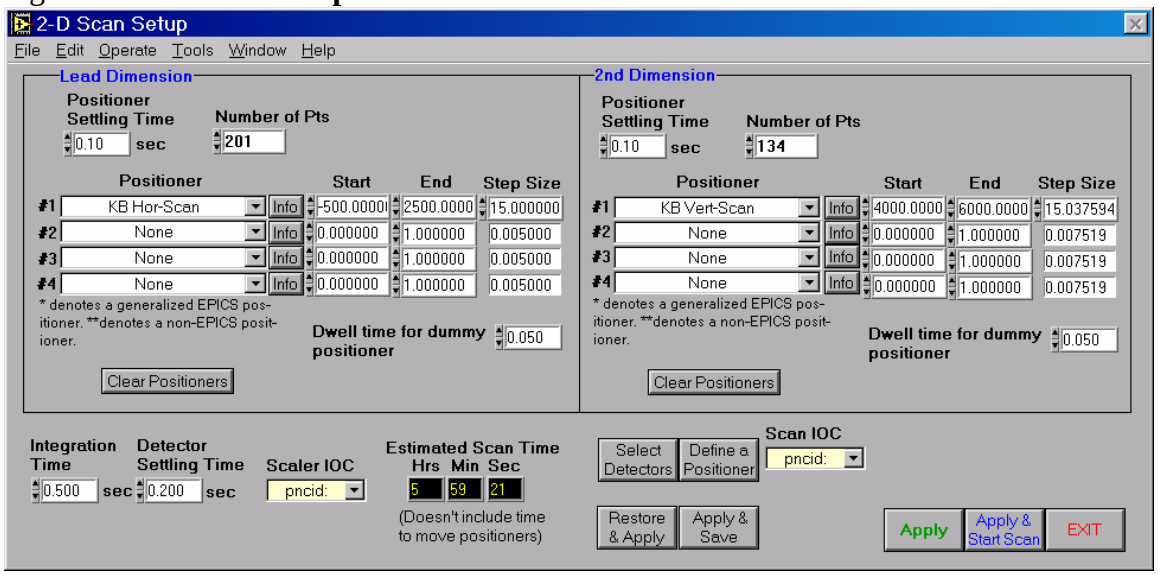
Action
Using 'Run Motor A.vi' and 'Run Motor B.vi' windows (Section 3.2) position the beam on the base-line left, base-line right, top left and top right corners in turn, of the rectangle to be mapped, and record in notebook the four co-ordinates on an annotated sketch.
Note that different motor selections within the 'Run Motor ...vi' window are associated with different units of measurement e.g. the 'B13-SampleHoriz' motor is measured in mm, whereas the 'KB Hor-Scan' (or the appropriate motor) which performs the same function is measured in microns.

Figure 4.2. 20 ID Control Panel v7b



Click on the up/down arrows on the 'Menu' box and select 'Data Collection'.
Click on '2-D Scan Setup'.

This takes the user to '2-D Scan Setup' window.
Figure 4.3**. 2-D Scan Setup**



In the 'Lead Dimension' box, set the 'Positioner Settling Time' at around 0.1 sec.
Under 'Positioner', click on the '#1' drop-down box and select e.g. 'KB Hor-Scan'.
Enter the x (horizontal) co-ordinates, with the left-hand vertical co-ordinate in the 'Start' column and the right-hand vertical co-ordinate in the 'End' column.

In the '2nd Dimension' box, set the 'Positioner Settling Time' at around 0.1 sec.

Under 'Positioner', click on the '#1' drop-down box and select e.g. 'KB Vert-Scan'. Enter the y (vertical) co-ordinates, with the base-line horizontal co-ordinate in the 'Start' column and the top horizontal co-ordinate in the 'End' column.

Note that you can use whatever motor or other control that is desired in the place of the KB controls mentioned above. In this way it is possible to make numerous kinds of 2D scans in addition to the physical scan of the sample described here.

The scan will then start in the base-line left corner and proceed through to the top right corner.

At the bottom of the '2-D Scan Setup' window, check the 'Integration Time' is around 0.1 sec (select time as appropriate for the sample), and the 'Detector Time' is around 0.3 sec.

Note that the 'Estimated Scan Time' is shown. The estimated time tends to be shorter that the actual time needed.

The scan time can be increased or decreased by

- ? by changing the 'Step Size' in the 'Lead Dimension' and '2nd Dimension' boxes (this alters the 'Number of Pts' recorded in that dimension),
- ? by changing the 'Number of Pts' (this alters the 'Step Size' in that dimension)
- ? by changing the total area of the scan by entering different co-ordinates.

Make the step sizes the same in the 'Lead' and '2nd Dimension' boxes.

Depending on the purpose of the scan, a larger, coarser grained map or a smaller, more finely grained map can be produced.

Click 'Apply' and then 'Exit'.

The scan will not yet proceed.

4.5. Produce MCA scan

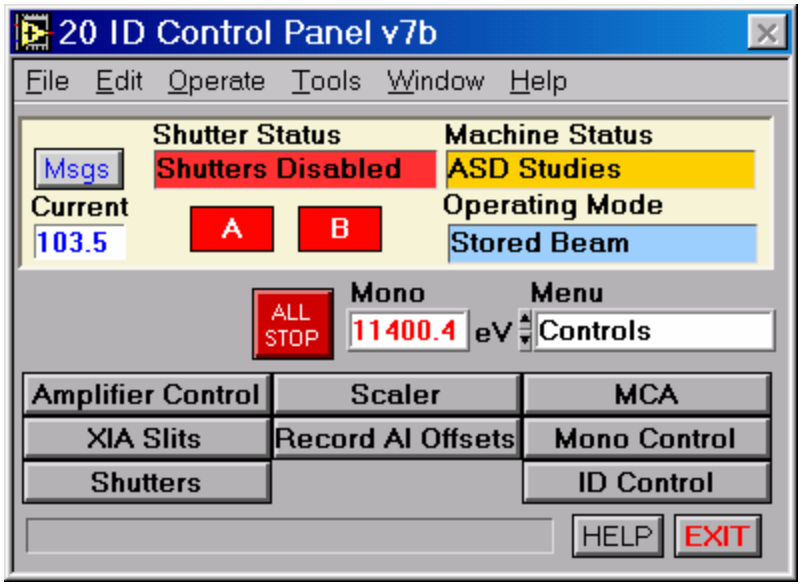
Reason

A MCA scan needs to be produced from a point on the sample to enable selection of the regions of interest (ROI), i.e. the range/s of the spectrum that encompasses the elemental peak/s the user has chosen to record and reproduce on the map.

Action

Position the beam on a spot (user choice) within the area to be mapped using 'Run Motor A.vi' and 'Run Motor B.vi' windows (Section 3.2) to adjust vertical and horizontal position.

Figure 4.5 **20 ID Control Panel v7b**



Click on the up/down arrows on the 'Menu' box and select 'Controls'.
Click on 'MCA' which takes the user to 'MCA Display v4b'

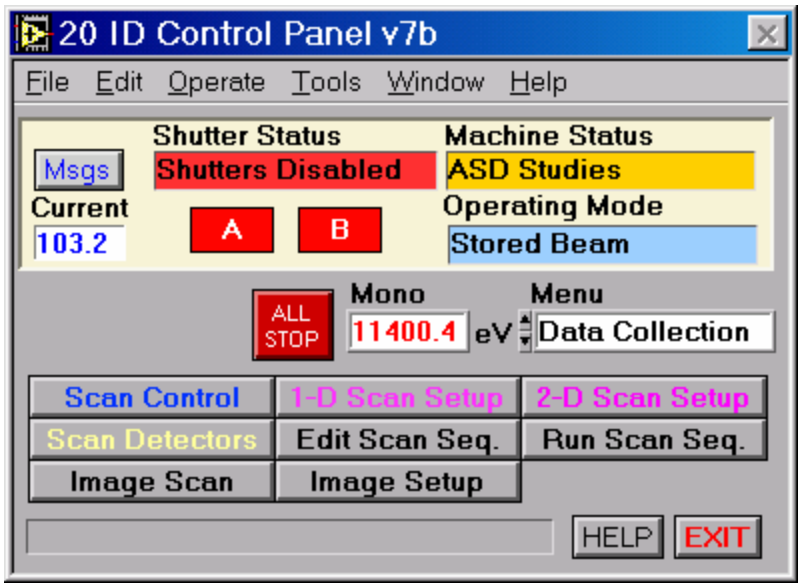
4.6. Select ROI

A MCA scan is collected and the ROI's are selected. The details of collecting a MCA scan and setting ROI's is in Appendix B2.3: MCA controls.

4.7. Produce Map

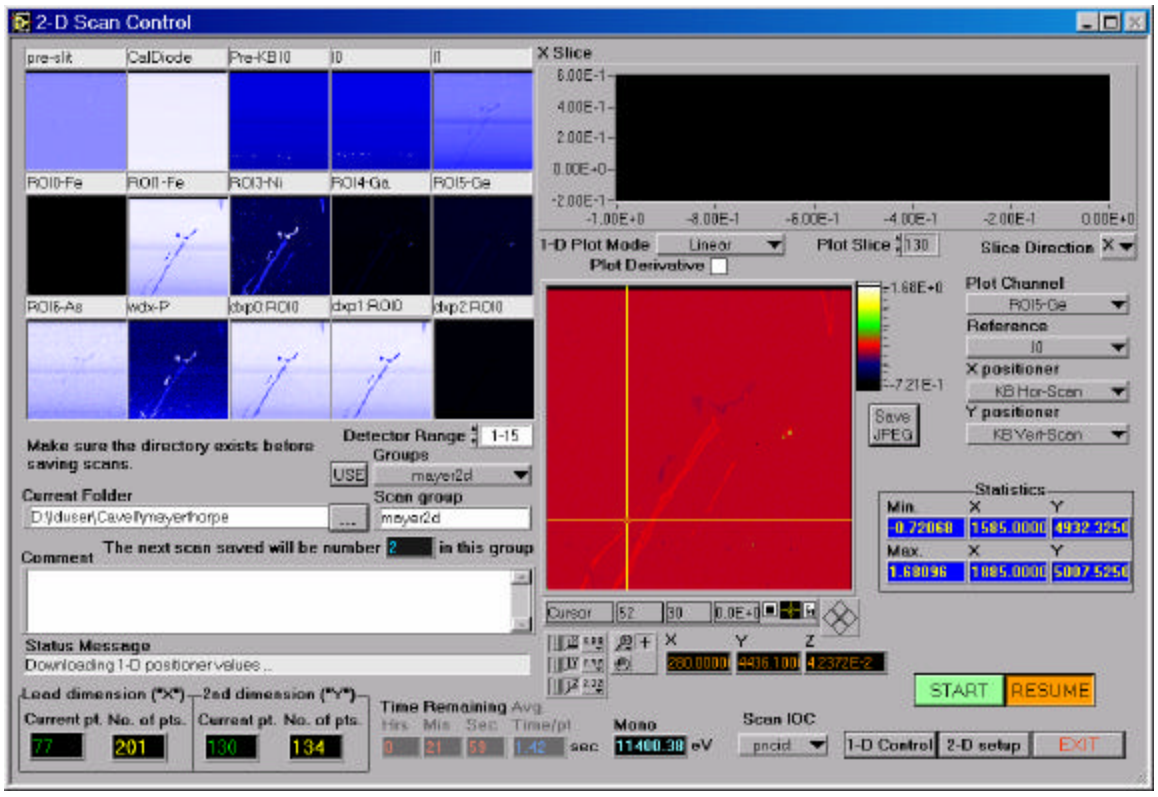
Use scan control to produce the map. Go back to 20 ID control panel and select 'Scan Control'

Figure 4.7.1: **20 ID Control Panel v7b**



You will then be asked to choose between 1D and 2D controls: select 2D (Apeendix B1.1). This will bring up the 2D control panel.

Figure 4.7.2 **2D Scan Control**



Choose the folder to put the spectrum in using the Current folder control. The Groups menu gives groups that are present in the folder or a new group can be entered under Scan group. Pressing 'enter' after typing a name in the scan group box will update the groups menu as well as select that group for the current scan group. The comment field can be used to add any comments to the saved file. It is a good idea to put information in the comments file such as the identity of the sample and the coordinates used for the map.

The boxes on the upper left will show the maps for each of the selected detectors. Note recent changes to the detectors may not be in the list but will be updated when the scan is started.

The field in the center shows the map as it is scanned. The map that is displayed is controlled by the pull down menus on the right hand side of the control panel.

The scan is started using the 'START' button. The scan can be paused and resumed using the 'PAUSE/RESUME' button. The 1-D control panel and the 2-D setup panel are accessed using the buttons in the lower right hand corner.

Appendix

A. CONTROL PANEL

The BM20 Control Panel window (see Fig. A1) provides access to all functions of the BL (NB. don't confuse this with the Windows Control Panel). The functions are organized into several categories, which are selected from the **Menu** list, as shown in Fig. A1.

Beamline Setup
Motors (rarely needed)
Displays (rarely needed)
Tables (rarely needed)

For each menu category, a new set of buttons comes up, which changes the appearance of the window drastically. Each of the buttons has an associated window or dialog box which comes up when you click the button. These are the same dialog boxes that are normally found scattered around the computer desktop. Therefore, if you close a dialog box by mistake, and want to reopen it, you can probably find it by looking carefully through the menu items on the Control Panel dialog box.

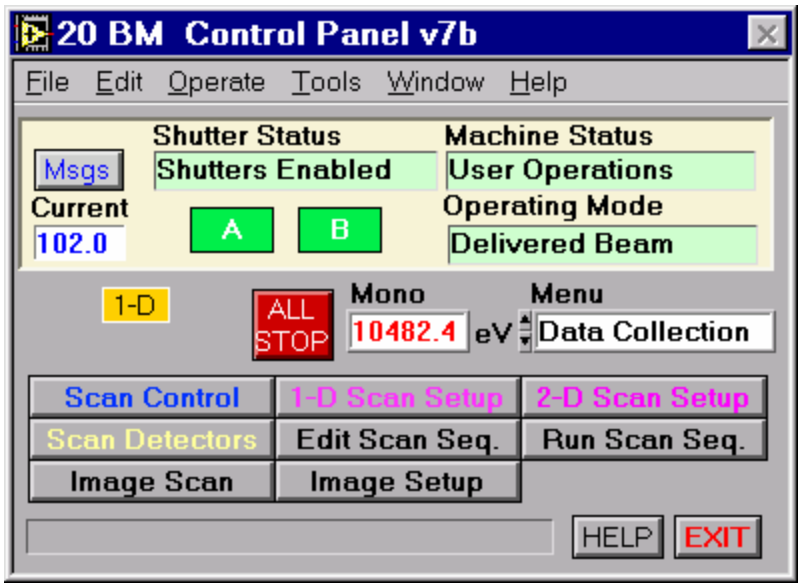


Fig. A1. BM20 Beamline Control Panel showing the Data Collection menu items as buttons (Scan Control etc.). The Control Panel buttons in themselves don't initiate any commands, so you can explore them without risk. In 2 or 3 cases, a warning box will come up telling you that something has not been set up. If in doubt, just exit. If the dialog box is already open somewhere it will be brought to the fore of the screen. The default virtual screen will also be displayed.

The ID20 Control panel is similar. And is used in the same manner as the BM20 control panel.

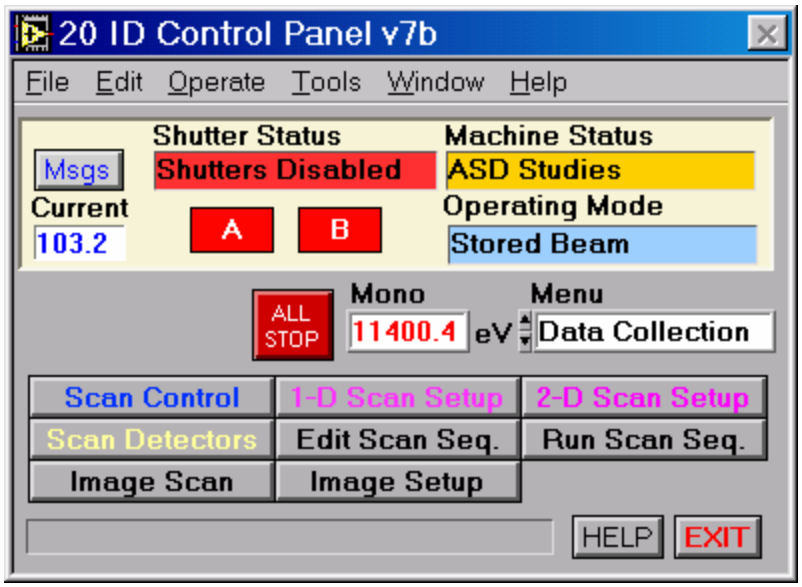


Figure A2. ID20 Control Panel showing Data Collection menu. The current beam status is shown here.

B. MENU ITEMS

The menu items in this section are found in the software on both beamlines. In some cases a panel may be labeled as BM or ID.

B1. DATA COLLECTION MENU

Fig. A1. Shows the appearance of the Beamline Control Panel when the **Data Collection** menu item is selected. The functions of the various buttons associated with this menu item are now summarized.

B1.1. Scan Control

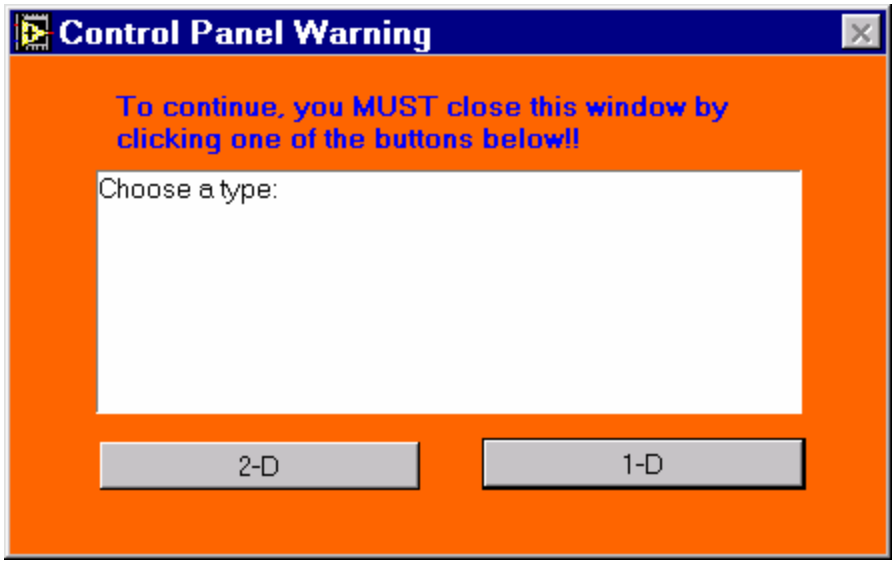


Fig. B1.1.

The '**Scan Control**' brings up a cryptic warning box, Fig. B1.1, which asks the user to select a 1D or 2D scan). On the BM station the 1D scan is typical while 2D is often used on the ID station.

B1.2. 1D Scan Setup

This button has the same function as the button with the same title which is found on the 1-D scan.control dialog, i.e. it brings up dialog box used to set up EXAFS/XANES scans (Fig. B1.2). See section 3.3 (above) for a description.

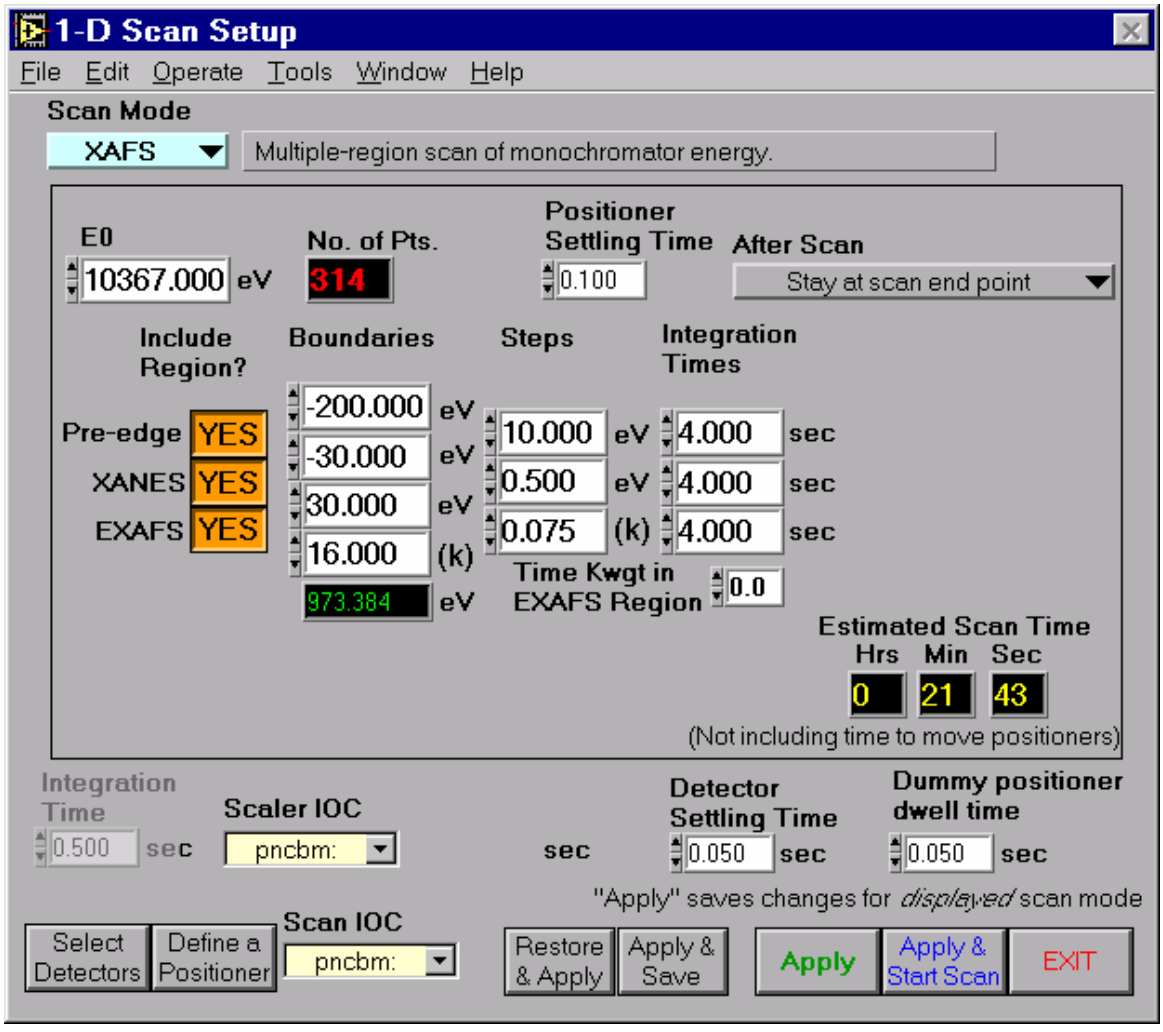


Fig. B1.2

B1.3. 2D Scan Setup

This is irrelevant for XAFS scans. The button brings up the window shown in Fig. B1.3 (which is used for imaging applications, Section 4.4).

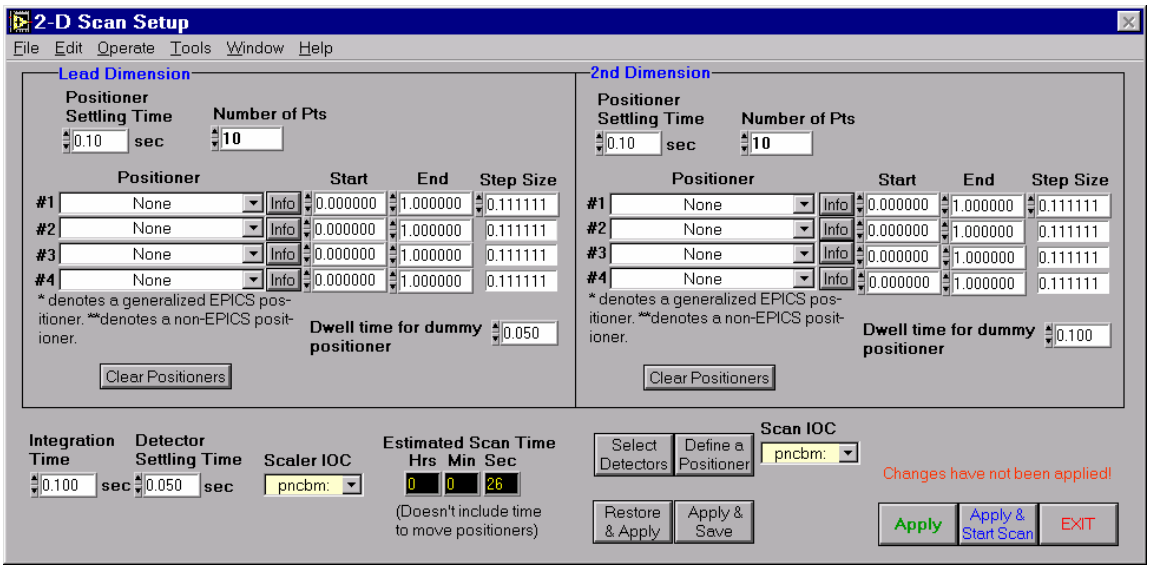


Fig. B1.3

B1.4. Scan Detectors

This button brings up a dialog box (**Scan Detector Selection**), Fig. B1.4, with a list of detector-derived quantities ('process variables') whose output can be selected for use in an XAFS scan. Various list-editing functions are provided by buttons on the dialog box. This window is used after a new detector has been installed.

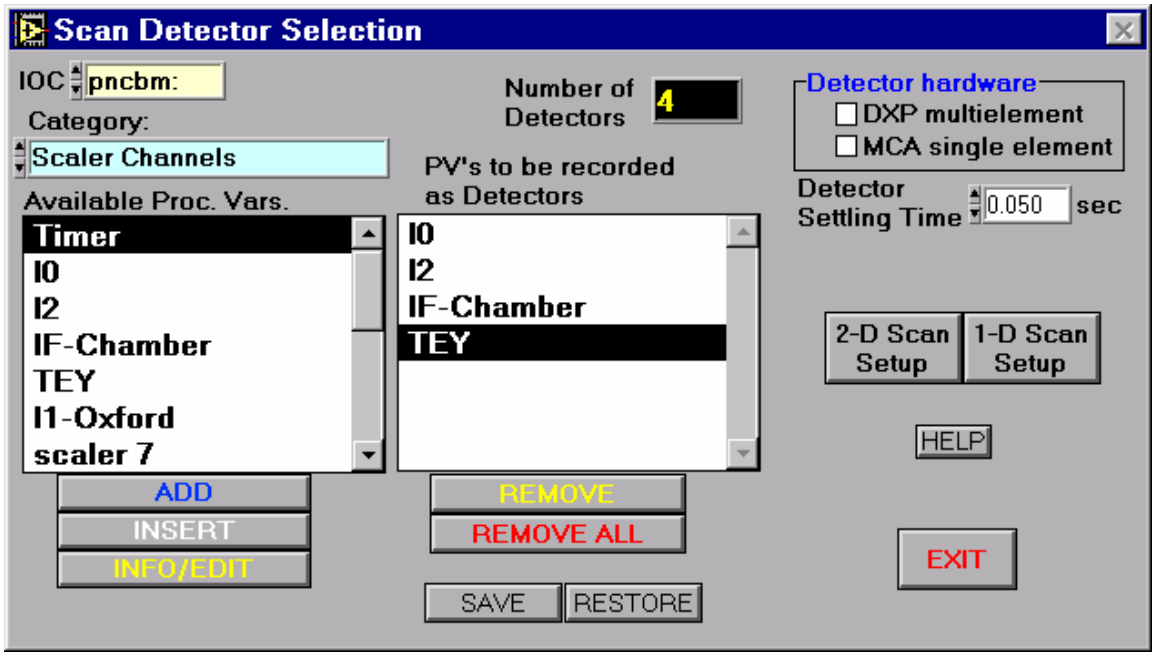


Fig. B1.4

The '**Scan Detectors**' is used to select which detectors are being used and direct the output of the detectors to the display and output file. The detectors are divided into categories and it may be necessary to search to find the desired detector. The desired detector is highlighted under '**Available Proc. Vars**' and the '**ADD**' button is pressed. This adds the detector to the '**PV**' list next to it. Note that the name put in the PV list is not necessarily the same as the detector name. The name in the PV list is edited by selecting the detector and pressing '**INFO/EDIT**'. The name chosen for the PV list will be the one used for display purposes and for labeling in the data file. It is best if the name chosen is somewhat meaningful to avoid confusion later on.

The UserCalcs (Appendix E) are selected here. A typical use is to use a UserCalc to take the output from each element of the 13 element detector and sum the signal for a particular ROI. In this case, it is useful to number the UserCalc and the ROI with the same number. It is also useful to name the PV with the element that was chosen.

B1.5. Edit Scan Sequence, Run Scan Sequence

These buttons bring up the dialog boxes used to program (Fig. B1.5.1) and execute scan sequences (Fig. B1.5.2). See section 3.8 (above) for description.

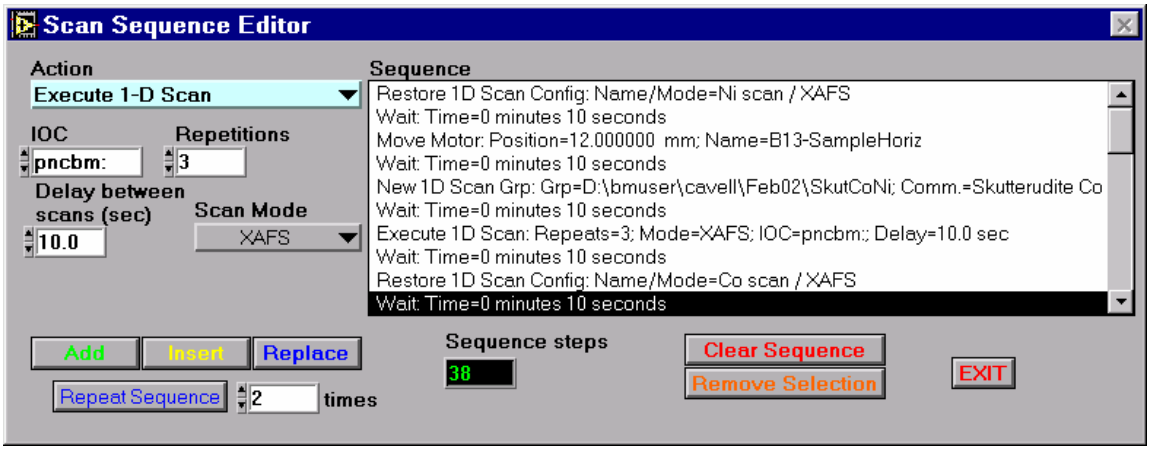


Fig. B1.5.1

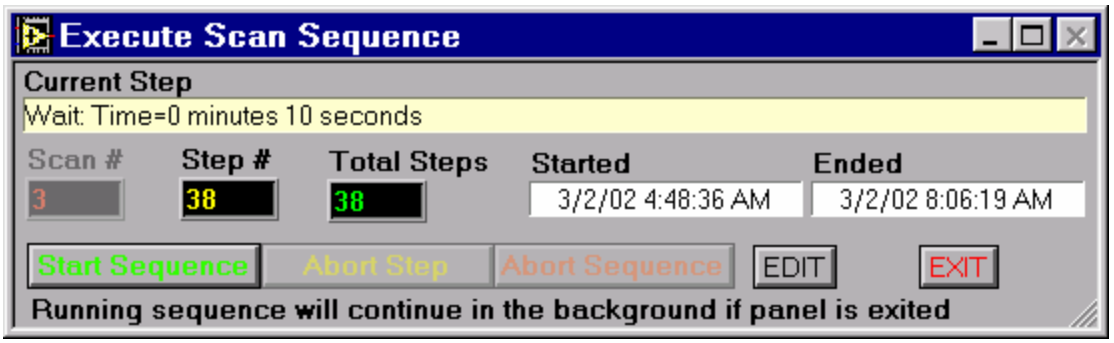


Fig. B1.5.2

B1.6. Image Scan and Image Setup

These functions refer to imaging applications. They are not used for XAFS scans.

B2. CONTROLS MENU

Fig. B2 shows the Beamline Control panel with the Controls menu item selected.

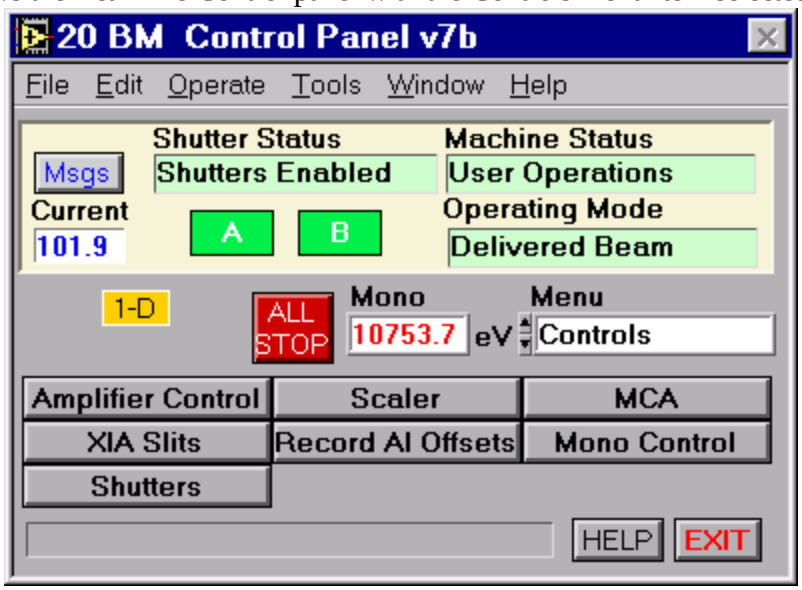


Fig. B2. Beamline Control panel with Controls menu item selected.

B2.1. Amplifier control

The associated dialog box is shown in Fig. B2.2. The controls are discussed in section 3.4 (above). You will probably get a warning if you have reason to open this dialog box for the first time (just ignore it).

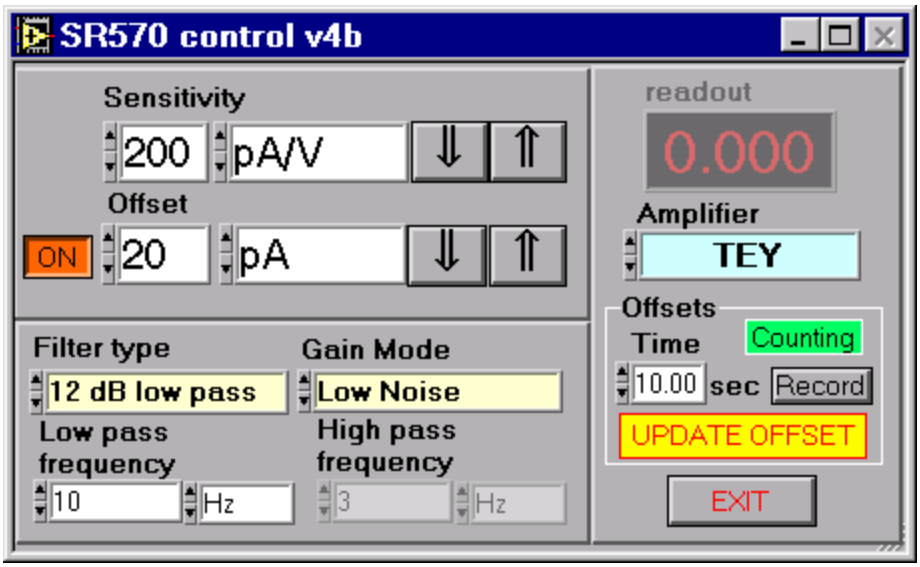


Fig. B2.1.

B2.2. Scaler control

This window (Fig. B2.2) is used by BL staff to define the quantities which constitute the measurable process variables. Once set, the general XAFS user should have no need to modify the parameters.

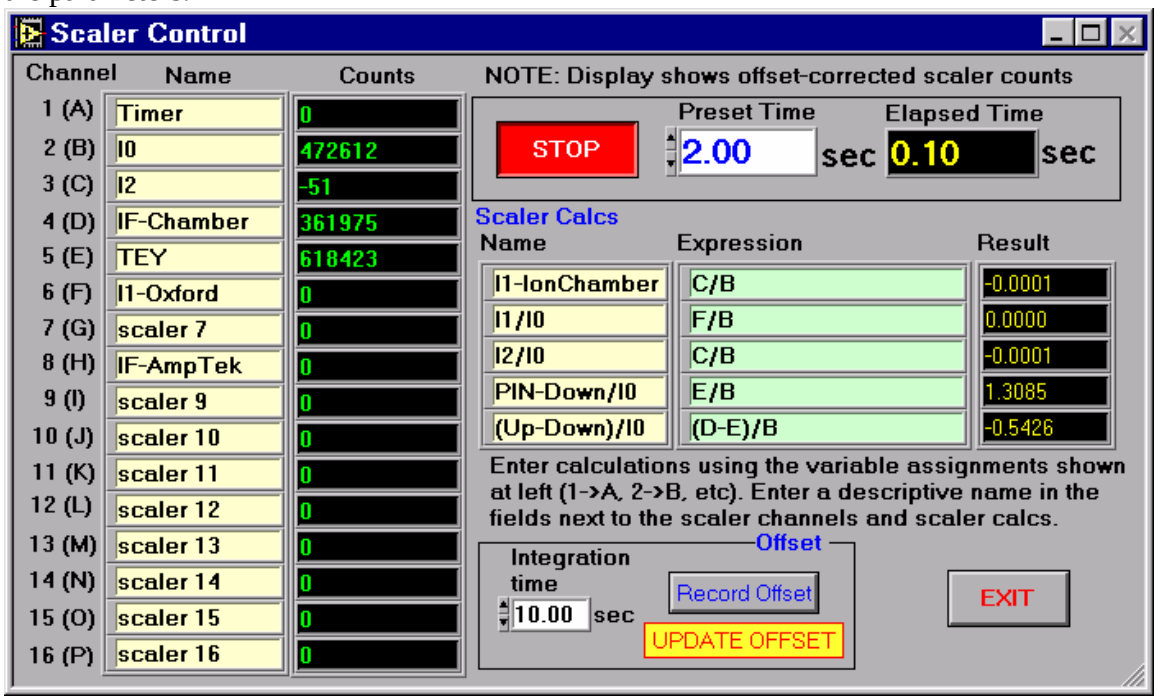


Fig. B2.2.

B2.3. MCA controls

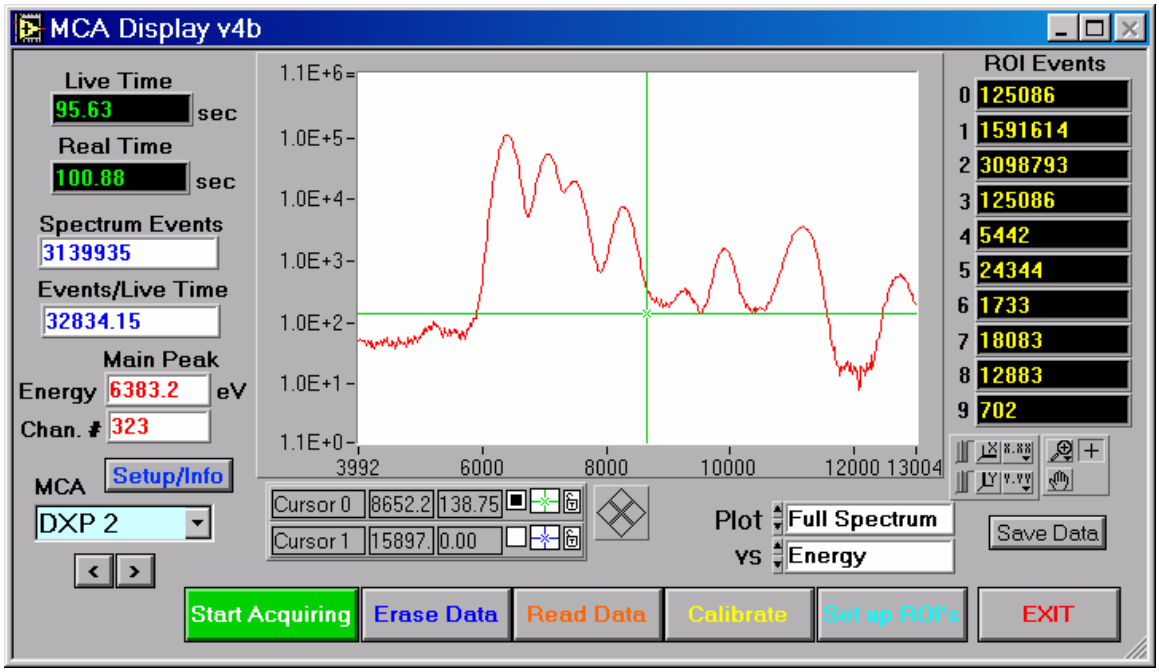


Fig. B2.3.1

The MCA controls shown in Fig B2.3.1 are used to run a MCA scan to set the ROI's for the solid-state detectors. Running a spectrum with the MCA is straightforward: select detector under **MCA**, click **Erase Data** followed by **Start Acquiring**. DXP 2 is the usual selection for the 13-element detector. Plot 'Full Spectrum vs Energy'. It takes ~60-300s to get a good spectrum. Keep the MCA screen open so you can check back: this screen is calibrated and shows energy as the scale.

The '**Live time**' and the '**Real time**' should be fairly close to each other. The 'Events/Live Time' shows you how much signal you are getting. For a map, a signal in the range of 50,000 to 75,000 is best. For an EXAFS scan a signal of less than 50000 works better to avoid saturation on the detector.

To set up ROIs hit the **Set up ROIs** button. The regions are defined by manipulating the positions of the vertical lines with the mouse.

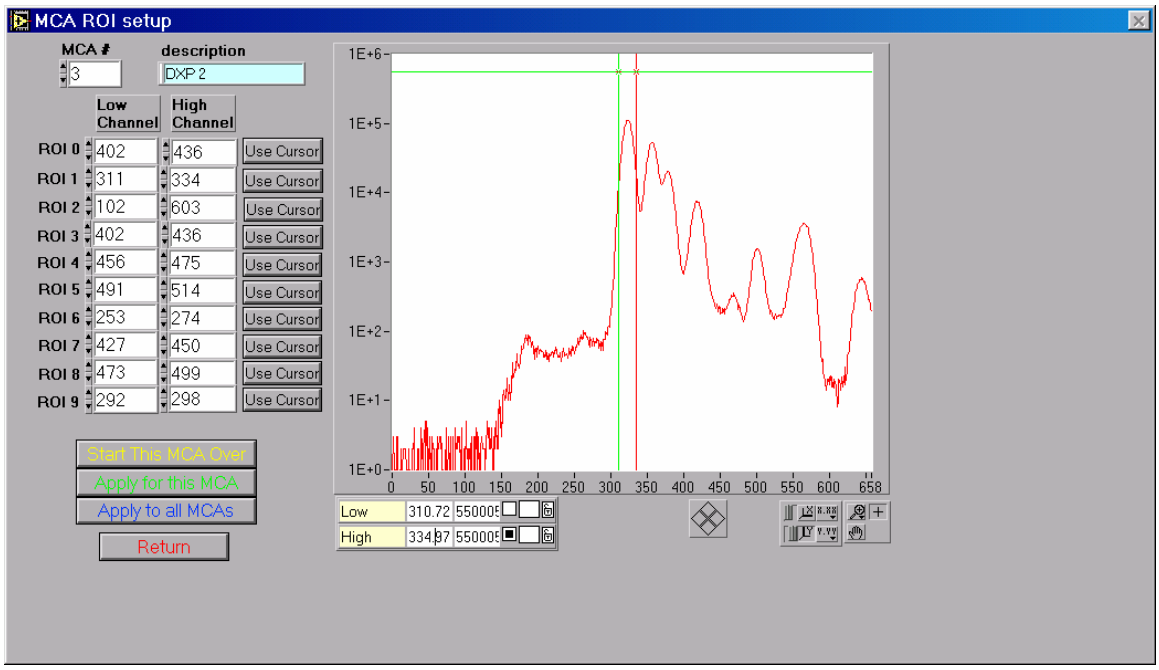


Fig B2.3.2

The green line defines the left edge and the red line defines the right edge. Note that you cannot move the left line past the red or vice-versa. When the area is selected a ROI is defined by pressing the '**Use Cursor**' button next to the desired ROI. The area can also be entered manually in to the 'Low Channel" and 'High Channel' columns. Each region of interest is set up in this manner. Note that the x-axis scale is not in energy but in channels. Refer to the previous panel for energy of each peak. Once all the regions are selected press the '**Apply to all MCAs**' button to apply the regions of interest. A small window will appear and ask which detectors to apply to. In general you want to apply to all detectors '**of this type**'. You will then return to the main MCA display.
CAUTION: The detector type is displayed under 'description'. Be sure that the correct detector is selected as the panel may start with a different detector than the one selected in the previous panel.

Note: Matching ROI numbers and UserCalc numbers is a good way to ensure that it is clear which UserCalc is being used for a particular ROI. Record the ROI's and the elements in your notebook.

It is possible to calibrate the energy scale in the main MCA panel. To do so press '**Calibrate**' in the main window. The calibrate window appears. For example to calibrate to a known peak, use the blue cursor to select a peak for which you know the energy value. The new energy is entered into the control box and press '**Calibrate**'.

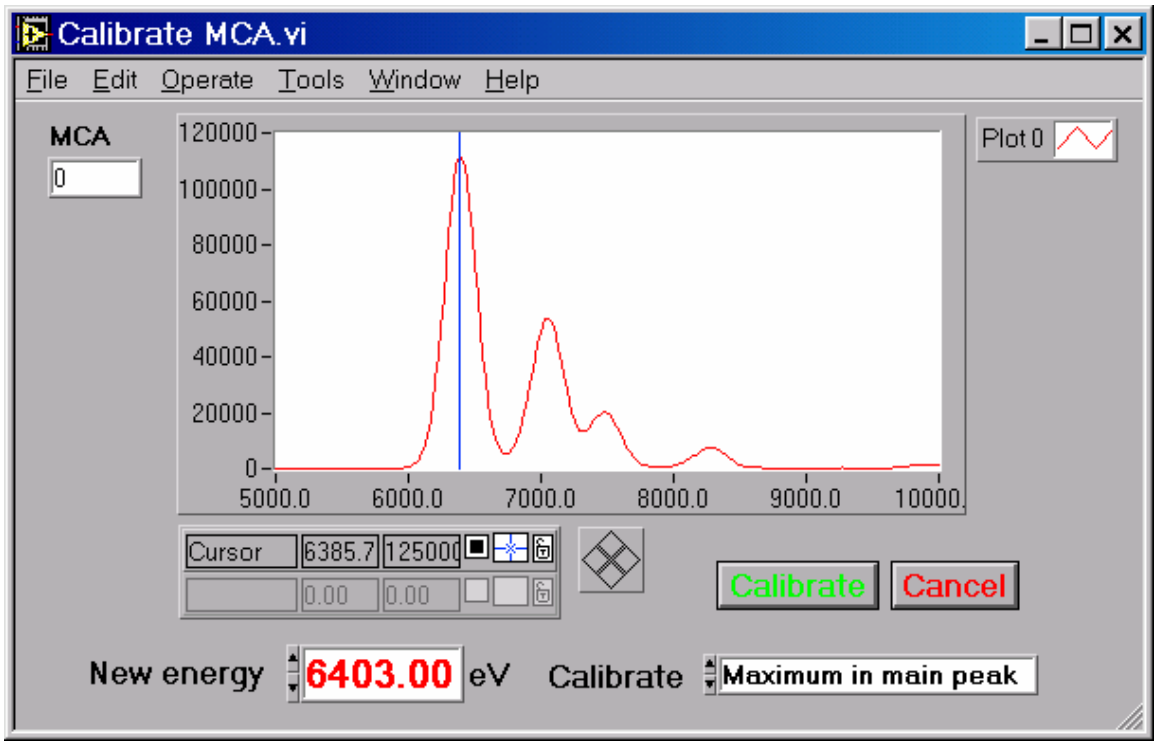


Fig B2.3.3

B2.4. XIA slits

Fig. A12 shows the XIA slit selection dialog box. The I_0 slits dialog box is what is normally needed, so click **OPEN** (or click exit to do nothing). This will bring up the slits dialog box shown in Fig. A13 which is discussed in section 3.1.

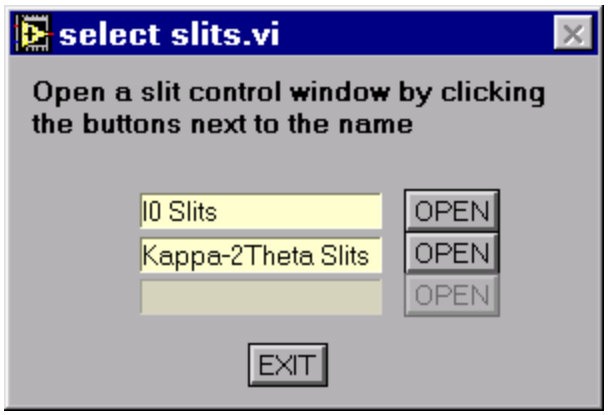


Fig. B2.4.1

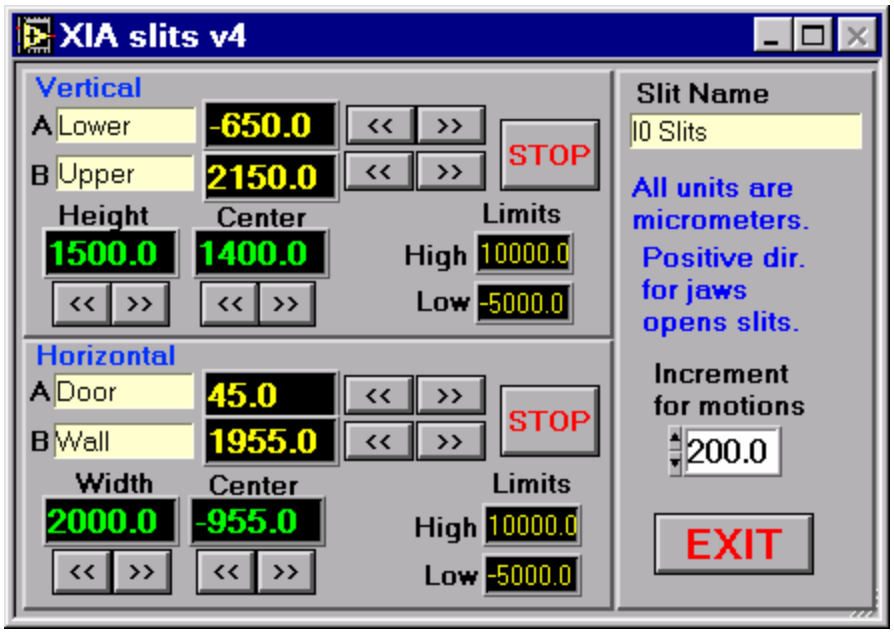


Fig. B2.4.2.

B2.5. Record AI offsets

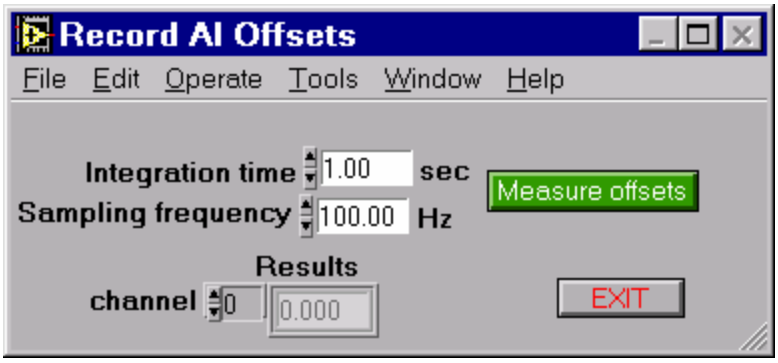


Fig. B2.5

The associated dialog box is shown in Fig. B2.5. It doesn't seem to be important.

B2.6. Mono Control

The Mono Control window is shown in Fig. A15. A description is given in section 3.4 (above).

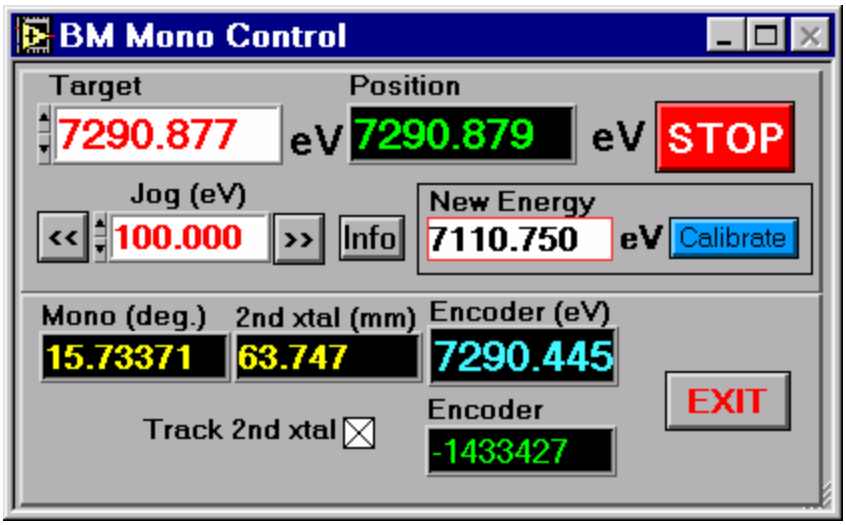


Fig. B2.6

B2.7. Shutters

Fig. A16 shows the Shutters control window. This window simply duplicates the function of the *real* shutters control buttons on the BL hutch wall. In general, there is no need for users to interact with this control window.

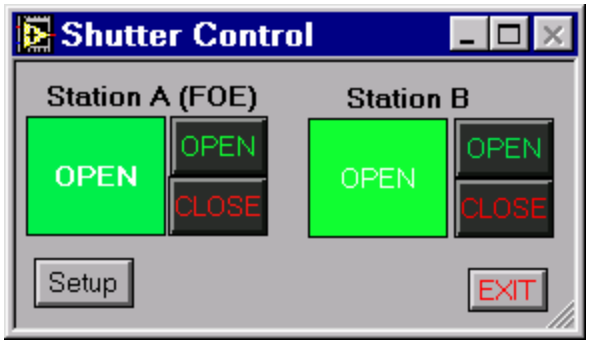


Fig. B2.7

B3. BEAMLINE SET-UP MENU

Fig. A17 shows the appearance of the Beamline Control Panel window when the Beamline Set-Up menu is selected. The **Analog Inputs** and **Pager** buttons can be ignored by the user, and are not discussed here.

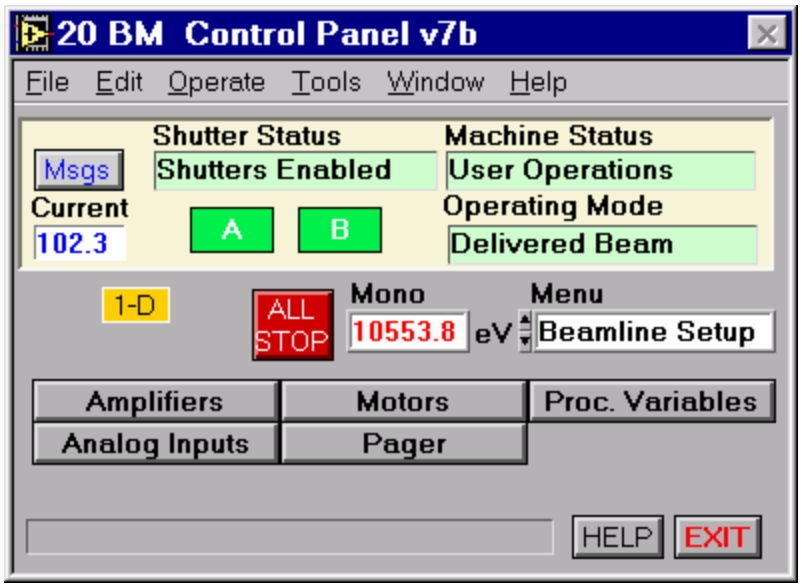


Fig. B3.

B3.1. Amplifiers

This window (Fig. A18) cannot be accessed while the **Amplifier Control** panel (sensitivity control, on Controls menu, Fig. A9). A warning message will advise you of this if you attempt to do so. You should not attempt to modify any parameters in the window without consulting the BL staff.

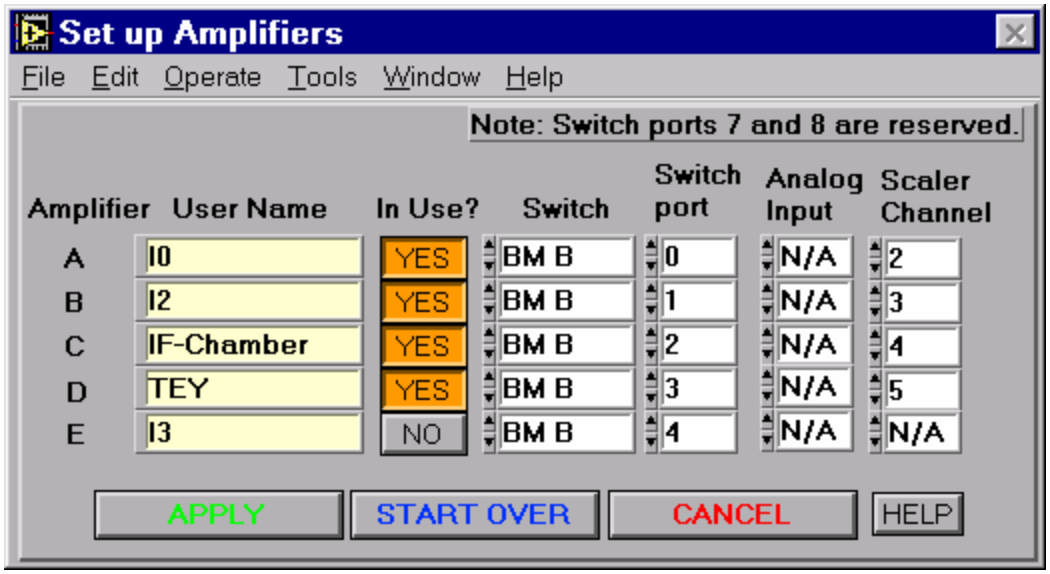


Fig. B3.1.

B3.2. Motors

The window which controls the sample position motors is shown in Fig. A19 and is discussed in section 3.2. There are several other types of motors in the system which are controlled by similar windows. Make sure you are moving the right one (often **B13 Sample Horiz** or **B14 Sample Vert**). The correct motor will depend on which beamline you are using as well as what it is you wish to move. You may need to consult with the BL staff to determine which motors you are using.

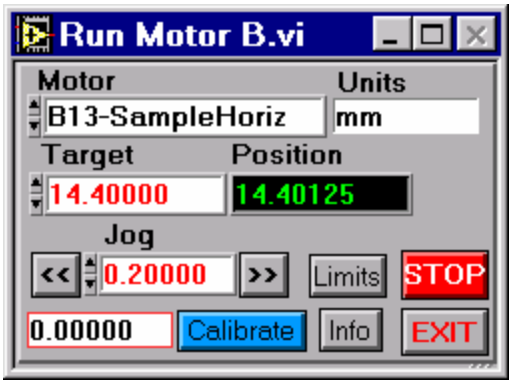


Fig. B3.2

B3.3. Process Variables

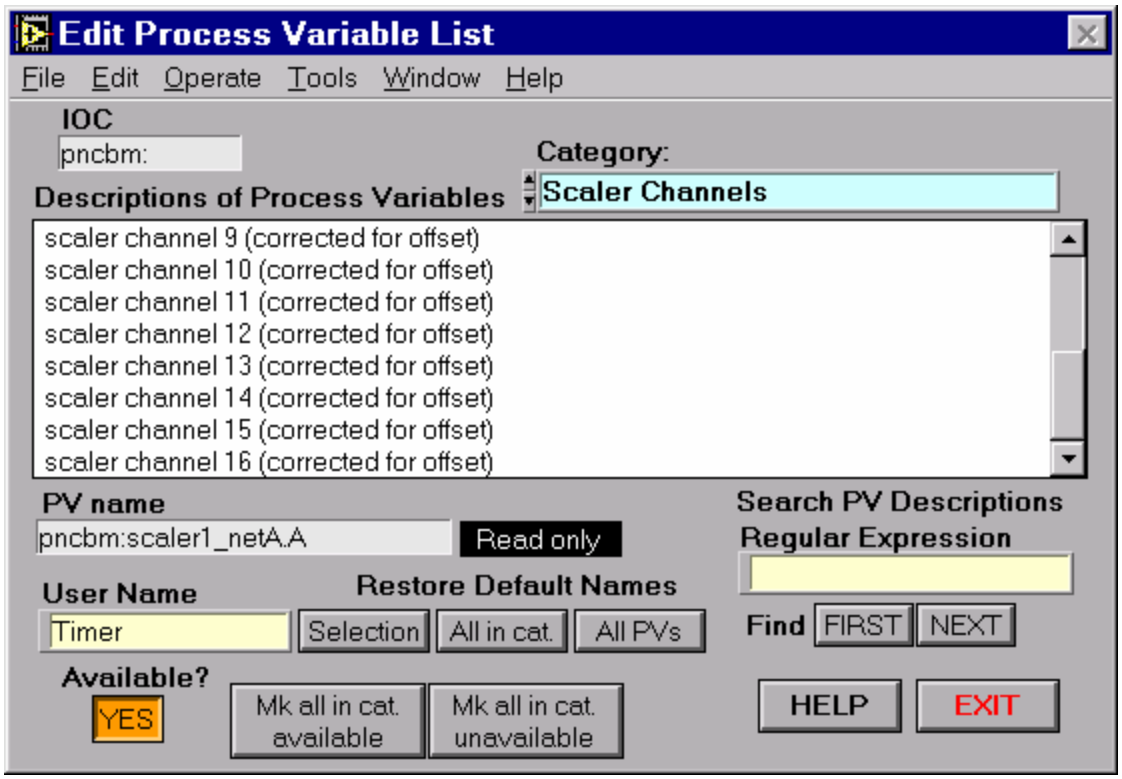


Fig. B3.3.

Fig. B3.3 shows the Process Variables window. This is yet another window used for interfacing output data to the computer control system. Users should not modify its settings without assistance from BL staff.

C. ID20 CONTROL PANEL

The ID20 Control Panel window (see Fig. A1) provides access to all functions of the BL. The functions are organized into several categories, which are selected from the **Menu** list, as shown in Fig. A1:

Data Collection
Controls
Beamline Setup
Motors (rarely needed)
Displays (rarely needed)
Tables (rarely needed)

For each menu category, a new set of buttons comes up, which changes the appearance of the window drastically. Each of the buttons has an associated window or dialog box which comes up when you click the button. These are the same dialog boxes that are normally found scattered around the computer desktop. Therefore, if you close a dialog box by mistake, and want to reopen it, you can probably find it by looking carefully through the menu items on the Control Panel dialog box.

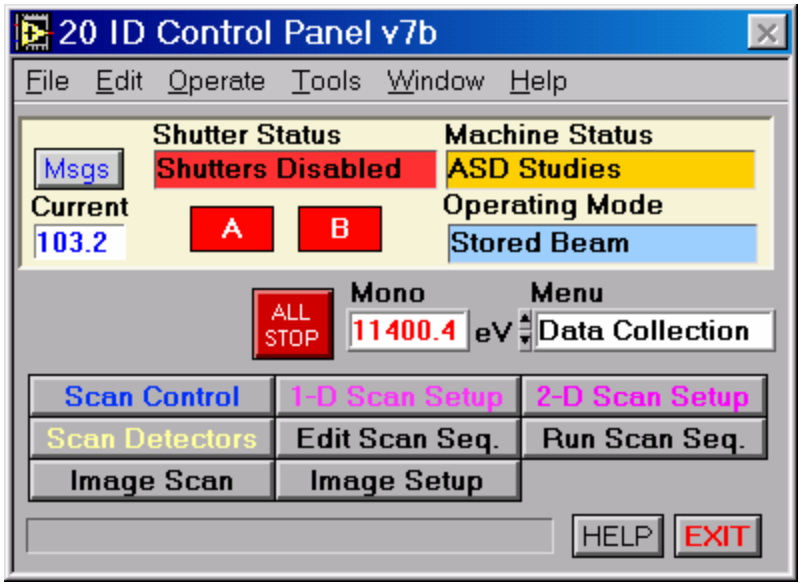


Fig. C1. ID20 Beamline Control Panel showing the Data Collection menu items as buttons (Scan Control etc.). The Control Panel buttons in themselves don't initiate any commands, so you can explore them without risk. In 2 or 3 cases, a warning box will come up telling you that something has not been set up. If in doubt, just exit. If the dialog box is already open

somewhere it will be brought to the fore of the screen. The default virtual screen will also be displayed.

D. Detuning

Adjusting the detuning (in the absence of the harmonic rejection mirror)
Detuning to 75% level is applied.

1) Set energy of interest in monochromator
2) Open slits (XIA) (especially vertical ones) to a wide value (~5000)
3) Make active (if necessary) motors for slits:
   - Beam position monitor (BPM) slit – upper
   - Beam position monitor (BPM) slit – lower

   Open these about 2mm each
4) Turn off feedback: Go to feedback set-up screen and press Pause
5) Note the I_0 value – reset the sensitivity to ~2-3 if necessary
   - Maximize with clockwise turns of the piezoelectric drive
   - Bring back in reverse direction to about 75% of the maximum I_0 value
6) Lower top and bottom BPM slits back into beam – step them into the beam in 0.2mm increments, one step in. Watch I_0 reading for indication that BPM slits are cutting beam. (Need a significant cut into the beam to get good signal into the feedback circuit otherwise oscillations arise.)
7) See new BPM set point value (on Feedback Display screen) – take this value and insert into (type into) space on Feedback Set-up screen.
8) Turn feedback on Resume
9) Restore XIA slits to previous (or new desired) value
10) Center the slit vertically especially if there has been a large shift in energy

Note that the ID beamline has both a vertical and a horizontal control which are both adjusted in a similar fashion. It is usually best to adjust the vertical and horizontal separately.

E. UserCalcs

UserClacs are defined to determine how the signals from the solid-state detectors are processed. Typically, a ROI for an element is summed up for each element of the detector to give a total signal. This may be divided by I0 automatically at this time if desired. The channels can also be averaged.

The UserCalcs are accessed using the Sun computer rather than the Labview program used for other tasks.

-each detector component is specified in a labeled line*

A pncaux:dxp_mca0.R1
(region of interest #1 for mca detector component “0”)
-
-
-
-
-
-
L pncaux:dxp_mca9.R1

-components say 0-12 except 11 (not working) and 9 (selected for ref later appears at end)

so: User Calc #1 = A+B+C+D+……+L

(note: in this case no normalization. Ratioing/subtraction/etc is applied. They may be if desired)

For another ROI say #2, starts all over
User Calc #2

A pncaux:dxp?mca0.R2
-
-
-
L 9.R2

A+B+C+D+….+L

Since .R1, .R2 is part of the PV name, there is no confusion

*order is not necessary but desirable for accuracy

User Calc limit: 10
Each user calc can have 12 items (if all 13 components were working one would have to be left out)

Making User Calcs:

Use Sun computer (sign on)
Bring up user calcs (on bmmain.adl)
Select on user calc with LH button – User Calc full
Screen comes up, edit as decided (see before)

Typ: 1/I0 TRIGGER – one must be triggered
Typ dxp 12 – yes
To transfer (activate) to list, which can be picked up by Labview controller press PROC for proceed. This then becomes defined.

Now to receive this data stream in Labview, go to detector list in appropriate Labview screen (where these user calcs just prepared have been added) and then add them into the active list.

Note: Sun Edit
The keys copy, cut and paste on keyboard work
To select, pointer must be on item
Pointer must not move out of box to copy, cut etc as desired
Move to new box, pointer with box, keep pointer in place, paste, ENTER
If not "ENTERED", item is not kept in new box